

朱传娴

客户顾问

hzhu@acsi.info

如何使用SciFinder获取科技信息

安徽师范大学

2016.09.13



提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

美国化学文摘社—Chemical Abstracts Service

- ACS的分支机构
- 创建于1907年，简称“CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市

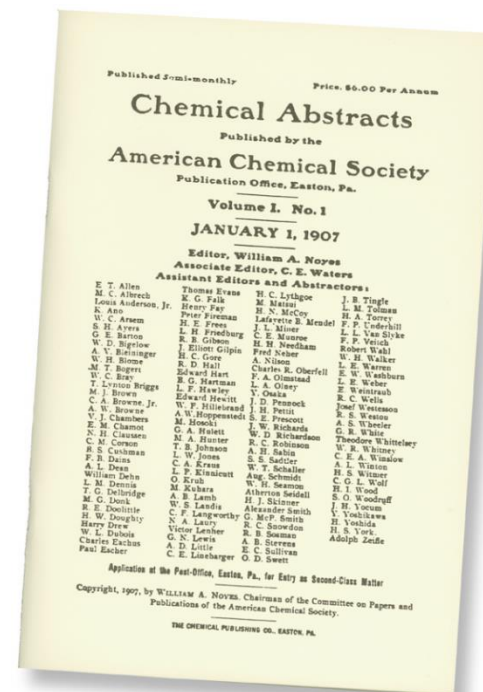


1907年，信息的汇集、管理发生了重大的变化



威廉·诺伊斯
(William A. Noyes)

- “化学文摘”创刊
- 当年编制近12,000条文摘
- 今天，CAS每年收录、创建来自期刊、专利和其他已公开信息的文摘达到了100余万条



CAS——构建最高质量的化学数据库



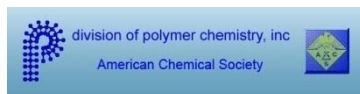
arXiv.org

Aldrichimica ACTA

ACS
chemical
biology



BEILSTEIN JOURNAL
OF ORGANIC CHEMISTRY



J | A | C | S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical
Neuroscience



THE JOURNAL OF
PHYSICAL CHEMISTRY
Letters

SCIFINDER[®]
A CAS SOLUTION

CAS——构建最高质量的化学数据库



CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水
染料、有机颜料;合成橡胶;纺织品、纤维

应用化学各领域：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

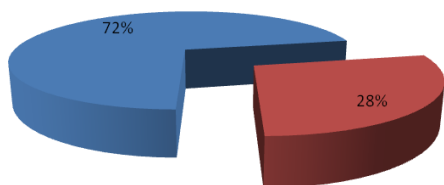
表面化学,催化剂,相平衡,核现象,电化学



CAS对各学科期刊文献的收录 (部分)

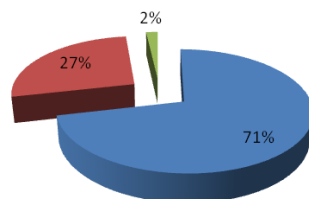
SciFinder收录材料学科期刊比例
(源自156份影响因子大于1的期刊)

■ CAPIus核心收录 ■ CAPIus收录 ■ 未收录



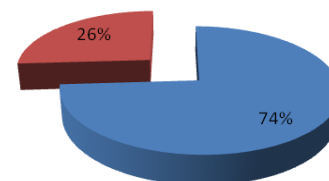
SciFinder收录化学工程学科期刊比例
(源自56份被SCI收录的期刊)

■ CAPIus核心收录 ■ CAPIus收录 ■ 未收录



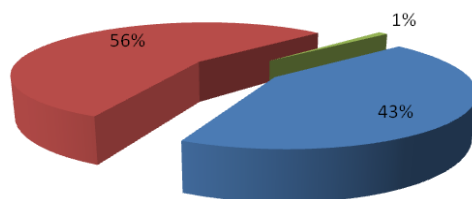
SciFinder收录环境化学期刊比例
(源自50份被SCI收录的期刊)

■ CAPIus核心收录 ■ CAPIus收录



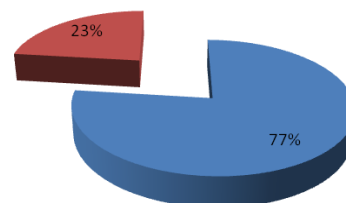
SciFinder收录药学类期刊比例
(源自166份被SCI收录的所有期刊)

■ CAPIus核心收录 ■ SciFinder收录 ■ 未收录



SciFinder收录生物化学类期刊比例
(源自26份被SCI收录的期刊)

■ CAPIus核心收录 ■ CAPIus收录



CAS数据库最具价值的内容——人工索引

4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751 PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014
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Indexing

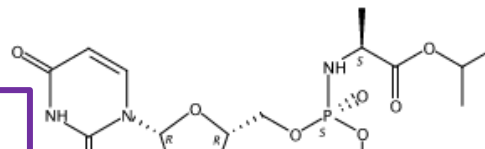
Carbohydrates (Section33-9)
Section cross-reference(s): 34, 63

Concepts

Crystallization	Drug bioavailability
Hepatitis C	Hepatitis C virus
Homo sapiens	Human
Pharmaceutical coated tablets	

Substances

[1190307-88-0P Sofosbuvir](#)  Page 2 in [PATENTPAK](#)
Absolute stereochemistry.



Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

CAS人工标引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term，CAS RN，CAS Role），提高效率，启发思路。

CAS最新动向—解决方案

PatentPak™

 **NCI™ Global**
A Solution Powered by CAS

 **METHODSNOW™**
A CAS SOLUTION

 **CHEMZENT™**
A CAS SOLUTION

 **SCIFINDER®**
A CAS SOLUTION

CAS最新动向—解决方案

- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息

6. Preparation of substituted nucleosides, nucleotides and analogs thereof as antiviral agents

Quick View PATENTPAK

By Beigelman, Le...
From PCT Int. App...

Patent No.	Kind	Language
WO 2016100441	A1	English

Disclosed he...
phosphate, R...
methods of t...
medicament

atkina, Natalia
Language: English, Database: CAPLUS

B is substituted purine and pyrimidine nucleobase; dashed bond between R and R' is absent, then R is H, substituted each R⁶ and R⁷ are independently hydrogen or deuterium; R⁵ is -OH or F; methods of synthesizing nucleotide analogs and as a HCV infection with one or more nucleotide analogs. Thus, nucleotide II was prepd. and tested as antiviral agent and of a hepatitis C virus.

7. Process for preparation of sofosbuvir

Quick View PATENTPAK

By Li, Zebiao; Zhu, Mingmin; Zhang, Qinghai; Zhu, Gongfeng; Zhang, Zhaoguo; Lin, Yanfeng
From Faming Zhuanli Shenqing (2016), CN 105669804 A 20160615. | Language: Chinese, Database: CAPLUS

The prep. method comprises reaction of (2'R)-2'-deoxy-2'-fluoro-2'-methyluridine with

ZOOM DOWNLOAD PDF

8. Q...
By F...

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

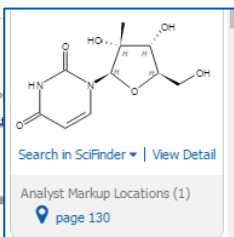
(43) International Publication Date
23 June 2016 (23.06.2016)

WIPO | PCT

(51) International Patent Classification:
C07H 19/10 (2006.01) C07H 19/13 (2006.01)
C07H 19/20 (2006.01) A61K 31/7072 (2006.01)
C07H 19/11 (2006.01) A61K 31/7076 (2006.01)
C07H 19/213 (2006.01) A61K 31/708 (2006.01)
C07H 19/067 (2006.01) A61P 31/14 (2006.01)
C07H 19/073 (2006.01)

(81) Designated States (kind of national protection):
AO, AT, AU, AZ, BA, BB, BG, BR, CA, CH, CL, CN, CO, CZ, DE, DK, EC, EE, EG, ES, FI, FR, GB, GR, HK, HU, IL, IN, JP, KR, LA, LC, LK, LR, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LU, MG, MW, MZ, NA, NG, SD, SI, SS, SZ, TZ, UG, ZM, ZW), EPO (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, JP, KR, LA, LI, LT, LU, LV, MA, MD, ME, MK, MN, MW, MX, MY, NZ, PA, PE, PG, PH, PL, PT, RU, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW).



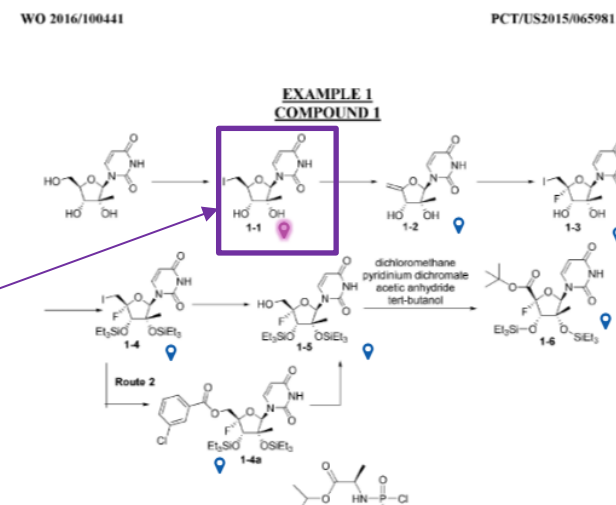
CAS RN 1206126-39-7

Search in SciFinder | View Detail

Analyst Markup Locations (1)
page 130

CAS RN 1206126-41-1

Analyst Markup Locations (1)
page 130



CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNow™
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求

SciFinder
SciPlanner
Reaction Structure substructure > reactions (9)
Analyze Reagent
1. View Reaction Detail
Single Step
Overview
Microcosm™
Procedure
1. Stir the mixture of 7-methyl-4-methoxy-2-methyl-2-oxo-1,4-dihydroquinoline-3-carboxylic acid (480 mg, 1.05 mmol), 1-iodooctane (388 mg, 1.82 mmol), copper(II) sulfate pentahydrate (42 mg, 0.17 mmol), (+)-sodium L-ascorbate (360 mg, 1.82 mmol) in t-BuOH/water (15 mL/15 mL) at room temperature for 4 hours.
2. Add water to the mixture.
View more...
Available Experimental Data
1H NMR, 13C NMR, IR, HRMS, Mass Spec, MP
View with MethodsNow

嵌在SciFinder中的合成模块

CAS Solutions
METHODSNow
atorvastatin
Results (528)
Sort Relevance
Analyte
Atorvastatin (227)
Atorvastatin calcium (211)
Ezetimibe (80)
Amlodipine besylate (56)
Fenofibrate (46)
View All
Matrix
Pharmaceutical tablets (293)
Blood plasma (60)
Tablets (49)
Pharmaceutical capsules (34)
Garcinia atroviridis (20)
View All
Method Category
Technique
Reversed-phase HPLC (152)
Spectrophotometry (101)
UV-visible spectroscopy (71)
HPLC (57)
Liquid chromatographic UV detectors (43)
View All
Analysis of Atorvastatin in Blood plasma by High-performance thin layer chromatography
CAS MN: 1-101-CAS-1389
View Details & Instructions
Add to Compare
Analyte Atorvastatin
Matrix Blood plasma
Other Materials Material: 60 F254 silica gel HP TLC plates
Method Category Active Pharmaceutical Ingredient and Metabolite Analysis
Technique High-performance thin layer chromatography
Equipment Used Automatic TLC Sampler 3
Source HPTLC determination of atorvastatin in plasma
Jamshidi, A.; Nateghi, A. R.
Chromatographia (2007), 65 (11/12), 763-766. Vieweg Verlag/GWV Fachverlag GmbH
Document Sources
Abstract

单独的分析界面

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciFinder覆盖的数据库



SciFinder登录网址: <https://scifinder.cas.org/>



Sign In

Username

Password

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(Do not use on a shared computer)

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What is SciFinder?

SciFinder[®] is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences.



News & Updates

Welcome to SciFinder

Did you notice our new look?
Our new branding will also be phased into training and other support materials in the coming months. If you are a Key Contact and have questions, or need assistance updating logos on any of your organization's websites, please contact the [CAS Customer Center](#).

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[New Commercial Source Logos](#)

输入SciFinder帐号和密码

SciFinder主界面

检索完，请点击退出

工具栏

The screenshot shows the SciFinder main interface. At the top left is the SciFinder logo with 'CAS Solutions' and 'A CAS SOLUTION' text. To the right of the logo is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner' buttons. Further right are links for 'Preferences', 'SciFinder Help', and a 'Sign Out' button. Below the navigation bar is a search area titled 'REFERENCES: RESEARCH TOPIC'. It features a search input field with example text: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. Below the input field is a blue 'Search' button and a link for 'Advanced Search'. On the left side, there is a sidebar menu with categories: 'REFERENCES' (containing Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (containing Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (containing Reaction Structure). On the right side, there is a 'SAVED ANSWER SETS' section listing various saved sets like 'CSF1R', 'jmc', 'EP 19870107847', etc., and a 'KEEP ME POSTED' section with a message 'You have no proxies.' and a link to 'Learn how to: Create Keep Me Posted'.

已保存的结果集

检索入口

定题追踪

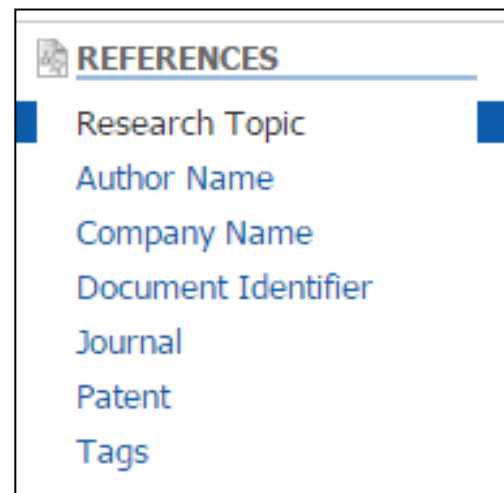
SciFinder检索——文献检索

■ 文献检索方法

- 主题检索
- 作者名检索
- 机构名检索
- 文献标识符检索
- 期刊名称和专利信息（公开号，申请号等）
- 从物质，反应获得文献

■ 检索策略推荐

- 关注某特定领域的文献：主题检索
- 关注物质有关的文献：先获得物质，再获得文献
- 关注某科研人员的文献：作者名检索
- 关注某机构科研进展：机构名检索



文献检索——主题

主题检索：纳米材料与基因的相互作用

检索式：Nanomaterial of gene



The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. A left sidebar contains three main categories: 'REFERENCES' (with sub-items: Research Topic, Author Name, Company Name, Document Identifier, Journal, Patent, Tags), 'SUBSTANCES' (with sub-items: Chemical Structure, Markush, Molecular Formula, Property, Substance Identifier), and 'REACTIONS' (with sub-item: Reaction Structure). The main content area is titled 'REFERENCES: RESEARCH TOPIC' and features a search input field containing the text 'nanomaterial with gene'. Below the input field, there are 'Examples:' listed as 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue 'Search' button is positioned below the examples, and an 'Advanced Search' link is located at the bottom of the search area.

关键词之间用介词连接：in, with, of...

主题检索的候选项

The screenshot shows the SciFinder interface with the search topic "Nanomaterial of gene". The results are displayed in a table with columns for selection, description, and the number of references. The second row is selected, indicating 633 references found containing both concepts closely associated.

		References
<input type="checkbox"/>	32 references were found containing "Nanomaterial of gene" as entered.	32
<input checked="" type="checkbox"/>	633 references were found containing the two concepts "Nanomaterial" and "gene" closely associated with one another.	633
<input type="checkbox"/>	2231 references were found where the two concepts "Nanomaterial" and "gene" were present anywhere in the reference.	2231
<input type="checkbox"/>	92865 references were found containing the concept "Nanomaterial".	92865
<input type="checkbox"/>	4508091 references were found containing the concept "gene".	4508091

Get References

“Concepts”表示对主题词做了同义词的扩展；

“Closely associated with one another”表示同时出现在一个句子中；

“were present anywhere in the reference”表示同时出现在一篇文献中；

按被引次数排序— Citing References

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'CAS Solutions', 'SCIFINDER A CAS SOLUTION', and user options like 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this is a secondary navigation bar with 'Explore', 'Saved Searches', 'SciPlanner', and action buttons 'Save', 'Print', 'Export'. The main content area shows a search for 'Nanomaterial of gene' with 510 references. A dropdown menu is open over the 'Sort by:' field, with 'Citing References' selected. The search results are listed in a table with columns for author name and citation count. The first three results are highlighted with a purple box, indicating they are the citing references. The first result is a review by Verma, Ayush; Stellacci, Francesco, titled 'Properties on Nanoparticle-Cell Interactions'. The second result is 'NanoGenotoxicology: The DNA damaging potential of engineered nanomaterials' by Singh, Neenu; Manshian, Bella; Jenkins, Gareth J. S.; Griffiths, Sioned M.; Williams, Paul M.; Maffei, Thierry G. G.; Wright, Chris J.; Doak, Shareen H. The third result is 'One-pot synthesis and bioapplication of amine-functionalized magnetite nanoparticles and hollow nanospheres' by Wang, Leyu; Bao, Jie; Wang, Lun; Zhang, Fang; Li, Yadong.

CAS Solutions | SCIFINDER A CAS SOLUTION | Preferences | SciFinder Help | Sign Out | Welcome Helen Zhu

Explore | Saved Searches | SciPlanner | Save | Print | Export

Research Topic "Nanomaterial of gene" > references (510)

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize | Sort by: Citing References | Accession Number | Author Name | Citing References | Publication Year | Title | Display Options

Analyze by: Author Name

Author Name	Citation Count
Qiu Jianying	37
Zhang Yunfu	37
Qiu Lin	36
Zhang Yuli	36
Chen Zhaoli	6
Jin Min	6
Qiu Zhigang	6
Shen Zhiqiang	6
Wang Jingfeng	6
Yang Dong	6

1. **Properties on Nanoparticle-Cell Interactions**
By Verma, Ayush; Stellacci, Francesco
From Small (2010), 6(1), 12-21. | Language: English, Database: CAPLUS

2. **NanoGenotoxicology: The DNA damaging potential of engineered nanomaterials**
By Singh, Neenu; Manshian, Bella; Jenkins, Gareth J. S.; Griffiths, Sioned M.; Williams, Paul M.; Maffei, Thierry G. G.; Wright, Chris J.; Doak, Shareen H.
From Biomaterials (2009), 30(23-24), 3891-3914. | Language: English, Database: CAPLUS

3. **One-pot synthesis and bioapplication of amine-functionalized magnetite nanoparticles and hollow nanospheres**
By Wang, Leyu; Bao, Jie; Wang, Lun; Zhang, Fang; Li, Yadong
From Chemistry - A European Journal (2006), 12(24), 6341-6347. | Language: English, Database: CAPLUS

Citing Reference: 帮助找到最重要的文献

文献检索结果

The screenshot displays the SciFinder interface with the following elements:

- Header:** CAS Solutions, SciFinder A CAS SOLUTION, Preferences | SciFinder Help, Sign Out, Welcome Helen Zhu.
- Navigation:** Explore, Saved Searches, SciPlanner, Save, Print, Export.
- Message:** 123 duplicates were automatically removed.
- Search Topic:** Research Topic "Nanomaterial of gene" > references.
- Tools:** Get Substances, Get Reactions, Get Related Citations, Tools.
- Actions:** Create Keep Me Posted Alert, Send to SciPlanner.
- Left Panel (Analyze by):**

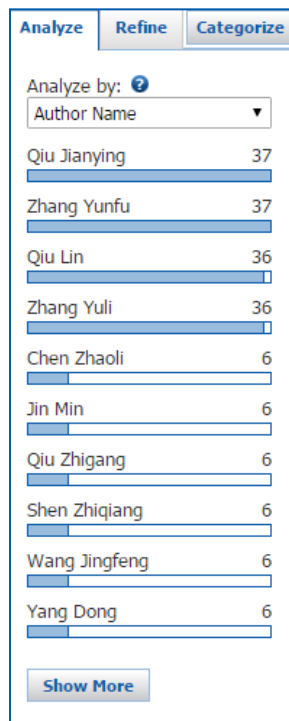
Author Name	Count
Qiu Jianying	37
Zhang Yunfu	37
Qiu Lin	36
Zhang Yuli	36
Chen Zhaoli	6
Jin Min	6
Qiu Zhigang	6
Shen Zhiqiang	6
Wang Jingfeng	6
Yang Dong	6
- Main Content:** 0 of 510 References Selected. Sort by: Accession Number. Three references are listed with titles like "Techniques for investigation and molecular toxicology of nanomaterials".

Annotations in Chinese:

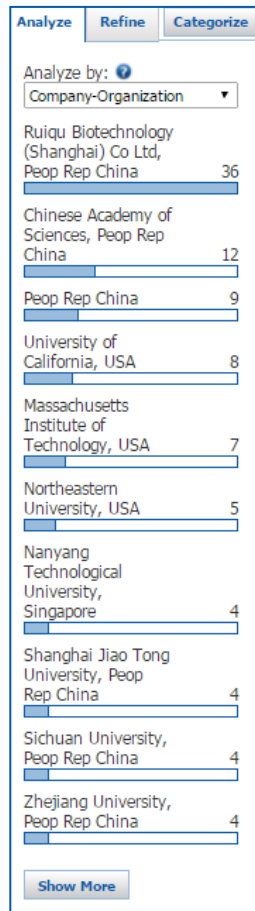
- 文献分析工具** (Literature Analysis Tool) points to the "Analyze" button.
- 获取原文** (Retrieve Original Text) points to the "Other Sources" link.
- A box at the bottom states: **SciFinder提供强大的文献处理工具，帮助处理文献** (SciFinder provides powerful literature processing tools to help process literature).

文献检索结果的Analyze

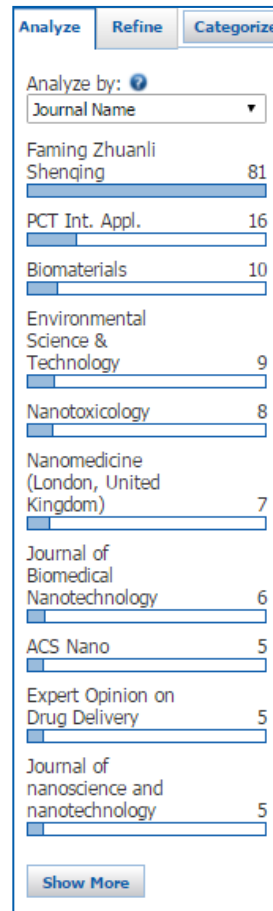
本领域研究人员



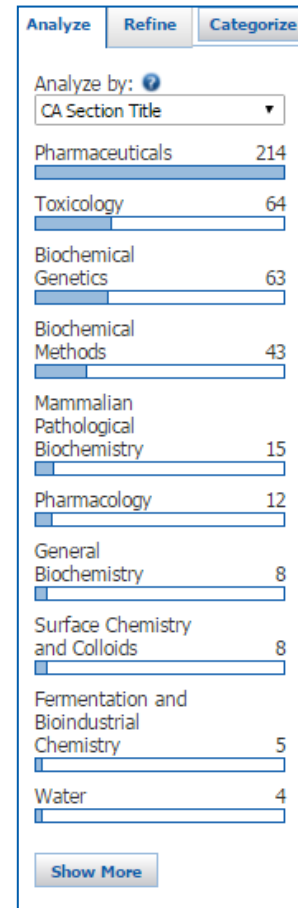
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期刊



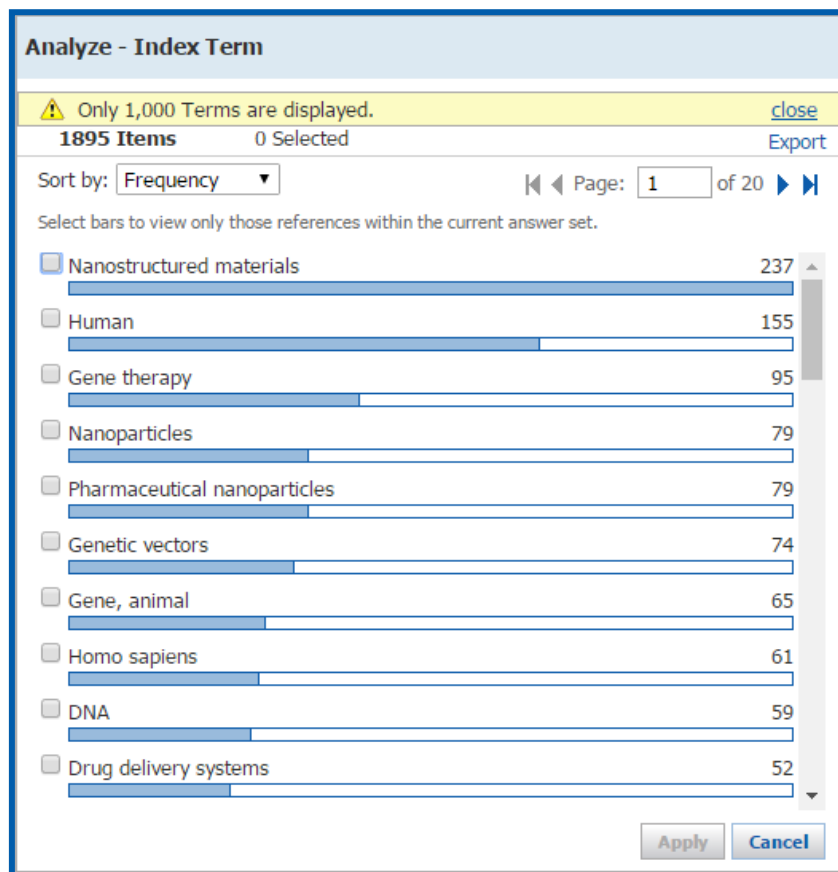
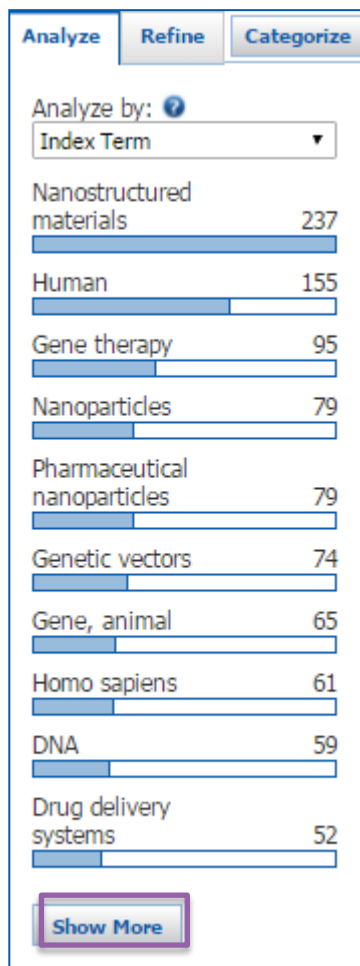
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文献检索结果的Analyze

Index Term :

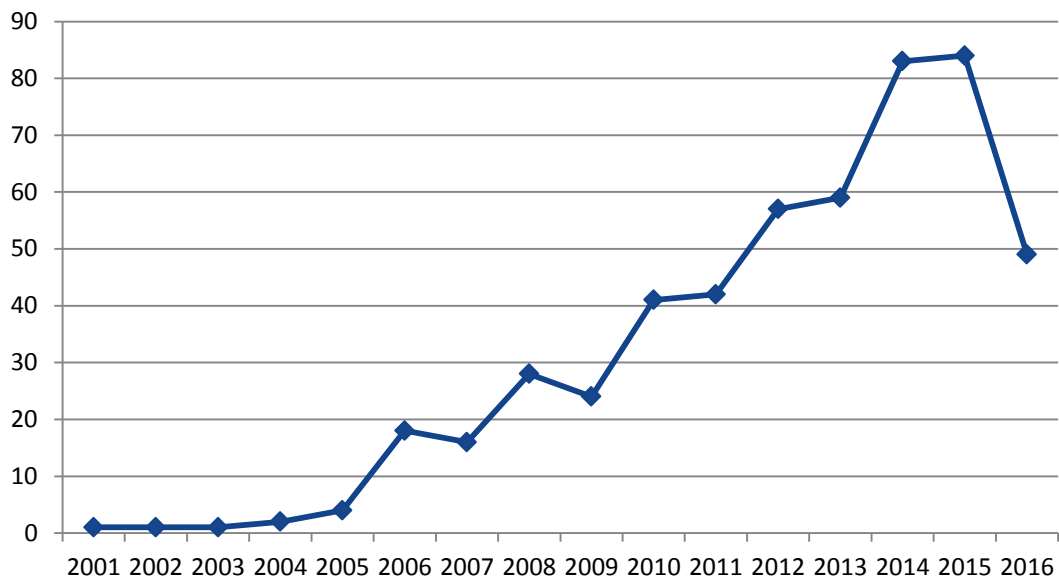
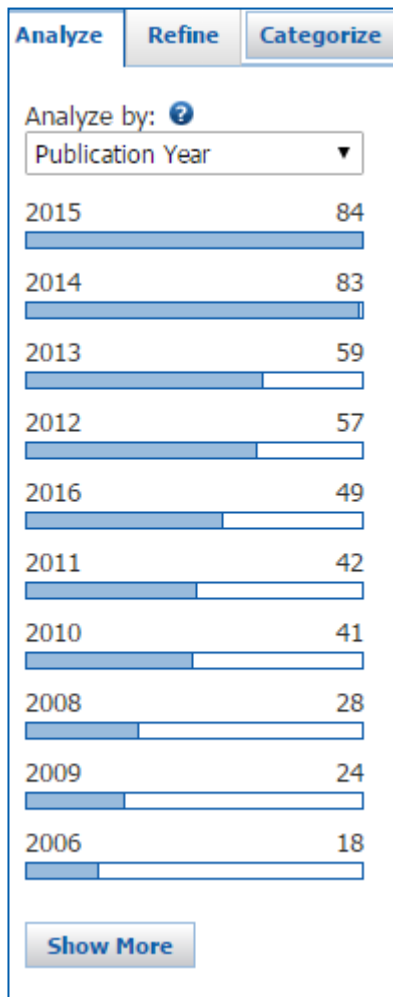
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- Author
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- Document Type
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Company Name

Examples:

3M

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Refine

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Sort by: Accession Number

0 of 170 References Selected

1. Techniques for investigating molecular toxicology of **nanomaterials**

Quick View Other Sources

By Wang, Yanli; Li, Chenchen; Yao, Chenjie; Ding, Lin; Lei, Zhendong; Wu, Minghong
From Journal of Biomedical Nanotechnology (2016), 12(6), 1115-1135. | Language: English, Database: CAPLUS

Nanotechnol. has been a rapidly developing field in the past few decades, resulting in the more and more exposure of **nanomaterials** to human. The increased applications of **nanomaterials** for industrial, com. and life purposes, such as fillers, catalysts, semiconductors, paints, cosmetic additives and drug carriers, have caused both obvious and potential impacts on human health and environment. Nanotoxicol. is used to study the safety of **nanomaterials** and has grown at the historic moment. Mol. toxicol. is a new subdiscipline to study the interactions and impacts of **materials** at the mol. level....

2. Preparation and application of recombinant plasmid loaded with polyethylene glycol-poly(lactic acid hydroxyl glycolic acid-polylysine composite **nano-material**

Quick View PATENTPAK

By Tang, Wei; Shi, Yongquan; Liu, Haoqi; Lv, Qian
From Faming Zhuanli Shengqing (2016), CN 105802981 A 20160727. | Language: Chinese, Database: CAPLUS

The present invention relates to the tech. fields of medicine and bioengineering, and specifically relates to a kind of recombinant plasmid loaded with polyethylene glycol-poly(lactic acid hydroxyl glycolic acid-polylysine composite **nano-material**, its prepn. method and application. The recombinant plasmid loaded with composite **nano-material** of the present invention is mPPP-pSNAV2-TGFβ1-IRES-TIMP1 (PSTIT); the present invention also provides the method for prepg. PSTIT, and its application in the prepn. of drug for treating diabetic foot (DF), and diabetics peripheral neuropathy (DPN). The prese...

3. Advances in researches on ecotoxic effects of manufactured **nanomaterials** on shellfish

Quick View Other Sources

By Ge, Chunmei; Huang, Xizhi; Lin, Daohui; Wang, Youji; Lu, Weiqun
From Shengtai Duli Xuebao (2015), 10(4), 1-16. | Language: Chinese, Database: CAPLUS

A review, with 76 refs., is given on advances in researches on ecotoxic effects of manufd. **nanomaterials** on shellfish. Nanotechnol. has become one of the most rapidly developing technologies in the 21 st century. **Nanomaterials** are widely applied to various areas because of the special phys. and chem. properties, including agriculture, electronics, biomedicine, manuf., pharmaceuticals and cosmetics, so **nanomaterials** are inevitably released into the aquatic environment. Shellfish has attracted much attention in **nano**-toxicol. studies due to its wide distribution, key position in food chain, fi...

4. Polymeric **nanostuctured materials** for biomedical applications

Quick View Other Sources

By Tang, Zhaohui; He, Chaoliang; Tian, Huayu; Ding, Jianxun; Hsiao, Benjamin S.; Chu, Benjamin; Chen, Xuesi
From Progress in Polymer Science (2016), 60, 86-128. | Language: English, Database: CAPLUS

Refine : 帮助用户迅速获得需要的文献

文献检索结果的Categorize

学科领域
主分类

学科领域
副分类

Index Term

选中的Index Term

Categorize ?

1. Select a heading and category.

Category Heading	Category
All	Substances in biological uses (449)
Genetics & protein chemistry	Substances in medicine (191)
Biotechnology	Medicine (103)
Biology	Toxicology & forensics (9)
Physical chemistry	Substances in adverse effects (10)
General chemistry	Agriculture (8)
Analytical chemistry	Food (6)
Technology	
Polymer chemistry	
Synthetic chemistry	
Catalysis	
Environmental chemistry	

2. Select index terms of interest.

Index Terms	Count
Page: 1 of 2	
Select All Deselect All	
<input checked="" type="checkbox"/> Gene therapy	34
<input type="checkbox"/> Molecular diagnosis	24
<input type="checkbox"/> Pharmaceutical nanoparticles	20
<input type="checkbox"/> Antitumor agents	17
<input type="checkbox"/> Cancer diagnosis	13
<input type="checkbox"/> Diagnosis	13
<input type="checkbox"/> Pharmaceutical carriers	10
<input type="checkbox"/> Drug delivery systems	7
<input type="checkbox"/> Polyethylene glycol	7
<input type="checkbox"/> Digoxin	6
<input type="checkbox"/> Ethanol	6
<input type="checkbox"/> Biocompatible materials	5
<input type="checkbox"/> Biomarkers	5
<input type="checkbox"/> Controlled-release drug delivery systems	4

Selected Terms

Click 'X' to remove the category from 'Selected Terms'

- Biotechnology > Medicine (1 Terms)

Biotechnology > Medicine > 1 Index Term(s) Selected

Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

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ally removed.

gene" > references (510) > refine "china" (170) > refine by categories

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0 of 34 References Selected Page: 1 of 2

1. Polymeric nanostructured materials for biomedical applications

Quick View Other Sources

By Tang, Zhaohui; He, Chaoliang; Tian, Huayu; Ding, Jianxun; Hsiao, Benjamin S.; Chu, Benjamin; Chen, Xuesi

From Progress in Polymer Science (2016), 60, 86-128. | Language: English, Database: CAPLUS

Polymeric nanostructured materials (PNMs), which are polymeric materials in nanoscale or polymer materials with tailored properties and functionalities for targeted biomedical applications. These materials, including micelles, dendrimers and nanocomposites, have been widely used in drug delivery, gene therapy, bio...

2. Powering up the molecular therapy of RNA interference by novel nanoparticles

Quick View Other Sources

By Liao, Wenzhen; Li, Wen; Zhang, Jiantian; Kirberger, Michael; Liu, Jun; Wang, Pei; Chen, Wei; Wang, Yong

From Biomaterials Science (2016), 4(7), 1051-1061. | Language: English, Database: CAPLUS

RNA interference technol. has been widely applied in biomedical therapy in recent years. A type of small RNA mol. - siRNA could regulate the expression of disease related genes by breaking down the integrity of mRNA with high specificity. However, the low efficiency of siRNA delivery to its target seriously hampered the RNAi therapy. Compared with viral-based delivery systems, non-viral-based nanoparticles are more suitable for disease treatment due to reduced cellular toxicity, higher loading capacity, and better biocompatibility. This review article highlights several nanoparticle-based ...

3. Cationic polymer nanomaterial gene vector and preparation method and application thereof

Quick View PATENTPAK

By Liu, Shangfeng; Li, Yongyong

From Faming Zhuanli Shenqing (2016), CN 105367781 A 20160302. | Language: Chinese, Database: CAPLUS

The invention discloses a cationic polymer nanomaterial gene vector and a prepn. method and application thereof. The vector is a copolymer core, a polylysine block (a) covalently connected to the polyethylene glycol core, a polylysine block and a polyhistidine block (b), or a random or a formed from lysine monomer, histidine monomer and optional amino acid monomer through polymn. The invention also discloses a compd. form nucleic acid, which is used for gene drug for treating tumor. The gene delivery vec...

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Example: 2-20

For: Citation Manager

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Offline review

Portable Document Format (*.pdf) Rich Text Format (*.rtf) Answer Keys (*.bt)

Saving locally

Answer Key eXchange (*.akx)

Details: File Name: * Reference_06_19_2012_100848

Format: Summary without abstracts Summary with partial abstracts Summary with full abstracts Detail (full record)

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Export Cancel

文献信息—题录、摘要、索引

3. Cationic polymer nanomaterial gene vector and preparation method and application thereof

By: Liu, Shangfeng; Li, Yongyong
Assignee: Peop. Rep. [China](#)

The invention discloses a cationic polymer nanomaterial gene vector and a prepn. method and application thereof. The vector is a copolymer comprising a polyethylene glycol core, a polylysine block (a) covalently connected to the polyethylene glycol core, a polylysine block and a polyhistidine block (b), or a random or alternate polymer section (c) formed from lysine monomer, histidine monomer and optional amino acid monomer through polymn. The invention also discloses a compd. formed with the copolymer and nucleic acid, which is used for prepg. drugs for treating tumor. The gene delivery vector not only can effectively deliver DNA, but also can effectively deliver RNA.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105367781	PATENTPAK	A	Mar 2, 2016	CN 2014-10443813	Sep 2, 2014

Priority Application

CN 2014-10443813	Sep 2, 2014
------------------	-------------

Indexing

Pharmaceuticals (Section63-6)

Section cross-

Concepts

重要概念

Antitumor agents
Genetic vectors
Homo sapiens
Nanostructured materials
Gene therapy
Hepatocellular carcinoma
Human
Neoplasm

Substances

重要物质

31961-02-1 Page 11 in PATENTPAK
cationic polymer nanomaterial gene vector and prepn. method and application for genetherapy of tumor
Reactant; Reactant or reagent

1885867-83-3DP deprotected carbobenzyloxy from Lys. Page 11 in PATENTPAK
cationic polymer nanomaterial gene vector and prepn. method and application thereof
Pharmacological activity; Properties; Synthetic preparation; Therapeutic use; Biological

QUICK LINKS

0 Tags, 0 Comments

PATENT INFORMATION

Mar 2, 2016
CN 105367781
A

APPLICATION

Sep 2, 2014
CN 2014-10443813

PRIORITY

Sep 2, 2014
CN 2014-10443813

SOURCE

Faming Zhuanli Shengqing
39pp.
Patent
2016
CODEN:CNXXEV

ACCESSION NUMBER

2016:348875
CAN164:409899
CAPLUS

LANGUAGE

Chinese

文献详情界面包括：

1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质，反应
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文献检索小结

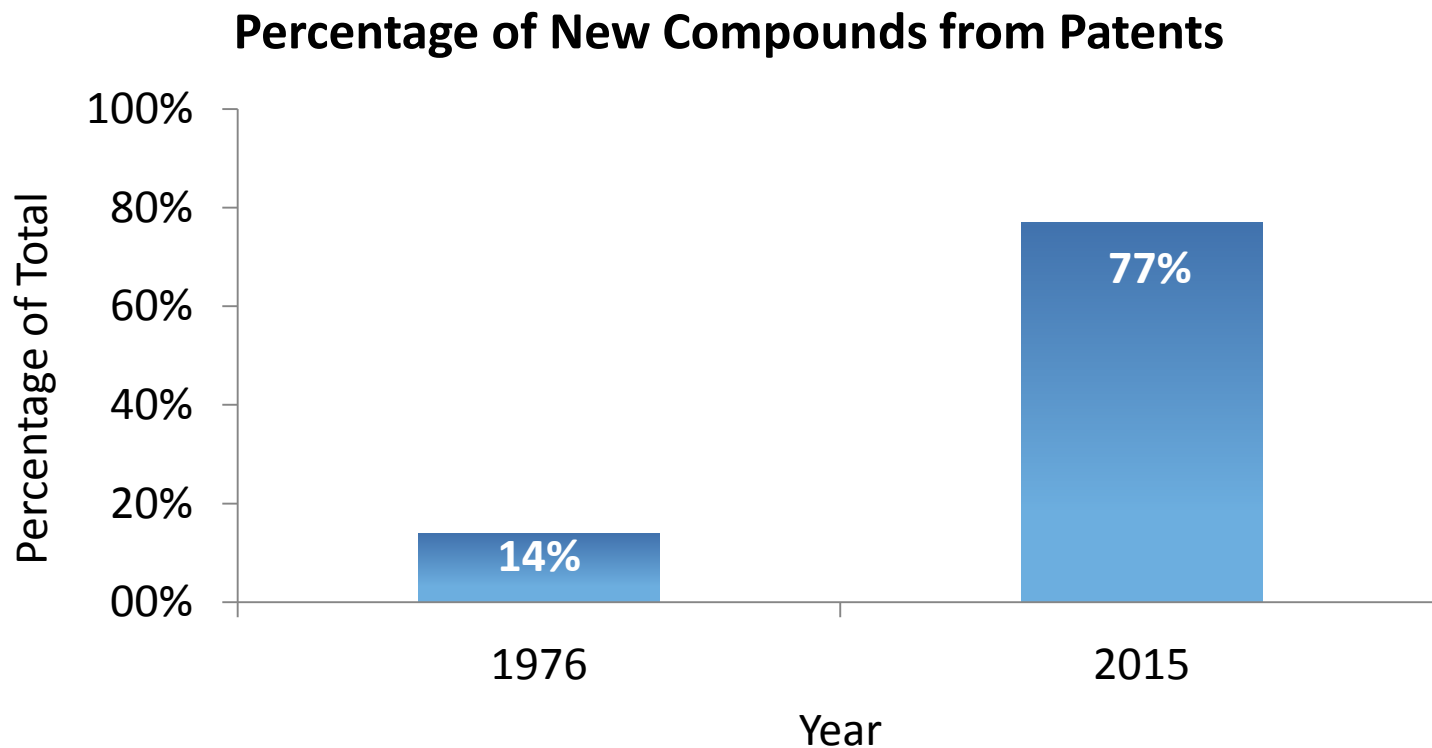
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PatentPakTM

专利工作流程解决方案



越来越多的新化合物倾向于首先通过专利公布



PatentPak——专利工作流程解决方案

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The claimed herbicidal formulations contain active ingredients from the group of N-(1,3,4-oxadiazol-2-yl)-arylcarboxylic acid amides (I; where A = N or C-alkyl, C-halogenalkyl, etc., R = alkyls, halogenalkyls, etc., X = alkyls and substituted alkyls, and Z = H, halogens, and substituted alkyls). The claimed amides can be formulated in mixts. with other herbicides and optional herbicide safeners. The herbicide combinations were evaluated against 15 test weeds. The herbicidal formulations are suitable for weed control in agricultural crops (esp. genetically modified crops) and other useful pl...

8. Preparation of 6-fluoro-9-methyl- β -carboline for the treatment of ear disease

Quick View

PatentPak

By Rommelspacher
From Eur. Pat. Appl.

Patent No.	Kind	Language
EP 2853533	Interactive	German

Patent Family

WO 2015044434	A2	German
WO 2015044434	A3	German

... methyl- β -carboline (I) and pharmaceutical compns. thereof useful in the treatment of acute and chronic inner ear diseases. ... 6-1-methyl-1H-Indole-3-ethanamine hydrochloride with 2,2-dihydroxyacetic acid followed by decarboxylation and redn. and

9. Preparation of fluoro-substituted 9-methyl- β -carbolines for the treatment of ear diseases

Quick View

PatentPak

By Rommelspacher, Hans; Enzensperger, Christoph
From PCT Int. Appl. (2015), WO 2015044434 A2 20150402. | Language: German, Database: CAPLUS

PatentPak——专利工作流程解决方案

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The screenshot displays the PatentPak interface. At the top, there are navigation controls for 'PAGE' (38 / 75) and 'ZOOM'. Two buttons, 'DOWNLOAD PDF' and 'LOAD PDF', are highlighted with a callout box. On the left, a sidebar shows 'Key Substances in Patent' with two entries: 'CAS RN 1689575-79-8' and 'CAS RN 24335-20-4', each with a chemical structure and a location marker for 'page 38' and 'page 60'. The main content area shows a patent document with a section titled 'Beispiele' and a sub-section 'Beispiel 1a: Synthese von 6-Fluor-9-methyl-β-carbolin'. A callout box points to a lightbulb icon in the text, indicating that clicking it will navigate to the PDF file's substance information.

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提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
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SciFinder检索选项——物质检索

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SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

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—有机化合物，天然产物：结构检索

—无机物，合金：分子式检索

—高分子化合物：分子式检索和结构检索

物质检索——标识符检索

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
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- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier**

REACTIONS

- Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER ?

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Examples:
50-00-0
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Acetaminophen

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1 3118-97-6

~894 ~58

CAS Registry Number: 3118-97-6

- » View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
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C₁₈ H₁₆ N₂ O
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

► **Key Physical Properties**
Regulatory Information
Spectra
Experimental Properties

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CAS Registry Number 3118-97-6

~894 ~58

C₁₈ H₁₆ N₂ O
2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

Molecular Weight
276.33

Melting Point (Experimental)
Value: 166 °C

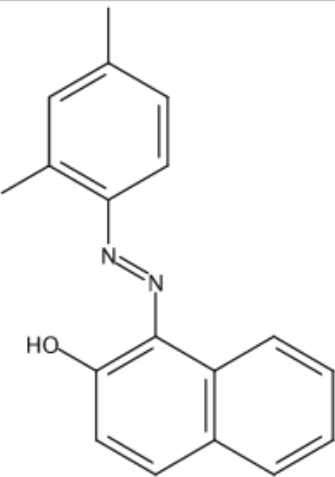
Boiling Point (Predicted)
Value: 476.7±40.0 °C | Condition: Press: 760 Torr

Density (Predicted)
Value: 1.14±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 13.52±0.50 | Condition: Most Acidic Temp: 25 °C

Other Names
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
AF Red No. 5
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The chemical structure shows a naphthalene ring system with a hydroxyl group at the 2-position and an azo group at the 1-position. The azo group is connected to a 2,4-dimethylphenyl ring.

物质详情

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<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses
<input type="checkbox"/> Occurrence	

For each sequence, retrieve:

Additional related references, e.g., activity studies, disease studies.

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生物研究

制备

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用途



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A CAS SOLUTION

EXPERIMENTAL PROPERTIES

实验数据与实验谱图

EXPERIMENTAL SPECTRA

¹H NMR IR Mass Raman UV and Visible

¹ H NMR Properties	Value	Condition	Note
Proton NMR Spectrum	See spectrum		(13)BIORAD

Notes

(13) BIORAD: Copyright Bio-Rad Laboratories. All Rights Reserved.

PREDICTED PROPERTIES

Biological Chemical Density Lipinski Structure Related Thermal

Lipinski Properties	Value	Condition	Note
Freely Rotatable Bonds	3		(21)
H Acceptors	3		(21)
H Donors	1		(21)
H Donor/Acceptor Sum	4		(21)
logP	5.471±1.252	Temp: 25 °C	(21)
Molecular Weight	276.33		(21)

预测数据与预测谱图

PREDICTED SPECTRA

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- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: PROPERTY

Experimental

Electric Conductivity (S/cm) ▾ > 353400
Examples: 44, 25-35, >125

Select Property...

- Boiling Point (°C)
- Density (g/cm³)
- Electric Conductance (S)
- Electric Conductivity (S/cm)**
- Electric Resistance (ohm)
- Electric Resistivity (ohm*cm)
- Glass Transition Temp. (°C)
- Magnetic Moment (μB)
- Median Lethal Dose (LD50) (mg/kg)
- Melting Point (°C)
- Optical Rotatory Power (degrees)
- Refractive Index
- Tensile Strength (MPa)

Examples: 44, 25-35, >125

寻找导电率比铜的60%大的非金属材料

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Property "Experimental - Electric Conduc..." > **substances (39)** > refine "exclude metal-containing" (14)

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- Chemical Structure
- Isotope-Containing
- Metal-Containing**
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Select One:

- Include only metal-containing substances
- Exclude metal-containing substances**

Refine

1. **1044804-35-4**

Substance
Image
Cannot Be
Displayed
1044804-35-4

Editor Note: A sulfonated polystyrene-doped PEDOT (H.C. Starck)

Unspecified
Clevios P-VP-AI 4083
Experimental Properties

2. **943433-94-1**

210531-45-6 (Component: 625392-06-5)
 $C_{13}H_8F_2O_7S_2 \cdot 2Na$

Click to view detail

0 of 14 Substances Selected

1. **1044804-35-4**

Substance
Image
Cannot Be
Displayed
1044804-35-4

Editor Note: A sulfonated polystyrene-doped PEDOT (H.C. Starck)

Unspecified
Clevios P-VP-AI 4083
Experimental Properties

Click to view detail

2. **868628-72-2**

$C_{18}H_{32}B N_2$
Boron, tributyl(1-(2-propen-1-yl)-1H-imidazole- κ^N)-, (7-4)-

Key Physical Properties
Experimental Properties

Chemical structure diagram of a boron complex with three tributyl groups and an imidazole ring.

3. **868628-71-1**

Chemical structure diagram of a boron complex with three tributyl groups and an imidazole ring.

4. **866023-23-6**

120120-58-3
 $C_{18}H_8O_4S_4$

Chemical structure diagram of a complex heterocyclic compound.

如何筛选非金属材料？

物质检索——分子式

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula**
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: MOLECULAR FORMULA

Examples:
H4SiO4
(C3H6O.C2H4O)x

Search

1. 151-21-3
(Component: 151-41-7)
~84904 ~276

• Na

C₁₂H₂₆O₄S.Na
Sulfuric acid monododecyl ester sodium salt (1:1)

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

金属盐：金属离子和阴离子间用点（.）分开

分子式输入需要遵守Hill排序规则：不含碳化合物，按元素符号的字母顺序排列；分子式为含碳化合物时，则“C”在前；如有氢则紧随其后，其它元素符号按字母顺序排在氢的后面

物质检索——结构

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure**
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:

Java Non-Java

Click to Edit

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

ChemDraw
Launch a SciFinder substance or reaction

Import CXF

Search

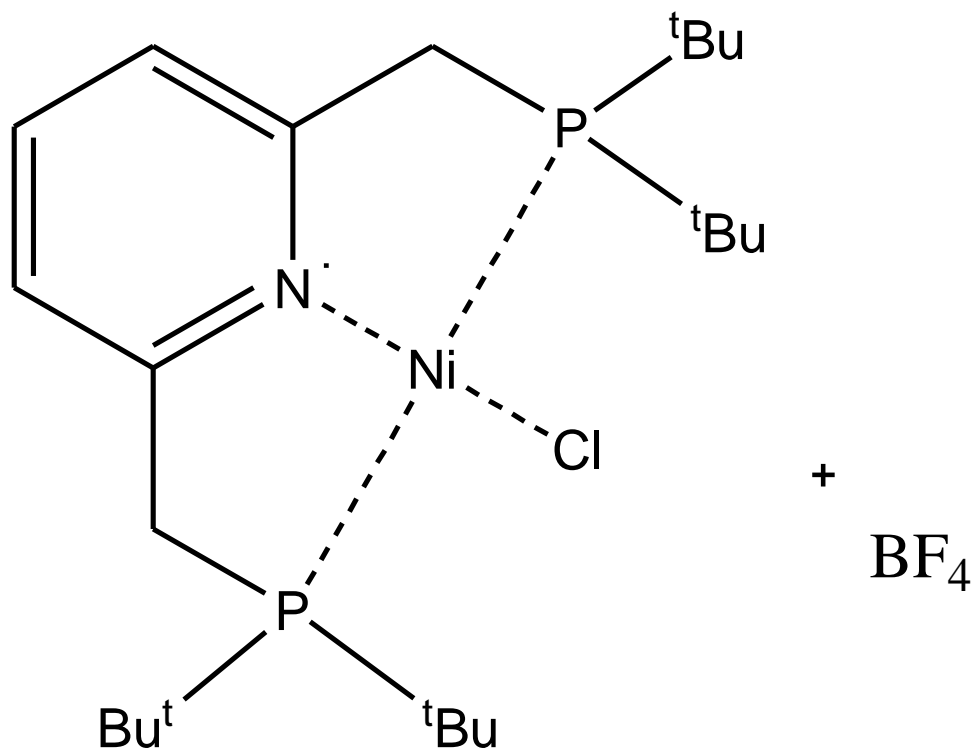
[Advanced Search](#) Always Show

物质检索——结构

The image shows a screenshot of the 'Structure Editor' software interface. The interface includes a toolbar on the left with various drawing and editing tools, a central workspace for drawing chemical structures, and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has radio buttons for 'Structure', 'Reaction', and 'Markush', and search options for 'Exact search', 'Substructure search', and 'Similarity search'. The interface also features a command line at the bottom with a chemical formula 'C H O S N P Cl Br F I Si' and a 'Scale 100' setting. The labels point to the following features:

- 橡皮 (Eraser)
- 结构和反应切换功能 (Structure and Reaction Switching Function)
- 铅笔 (Pencil)
- 元素周期表 (Periodic Table)
- 可变基团 (Variable Group)
- 重复基团工具 (Repeat Group Tool)
- 碳链工具 (Carbon Chain Tool)
- 选择工具 (Selection Tool)
- 环锁定工具 (Ring Locking Tool)
- 旋转工具 (Rotation Tool)
- 正电子 (Positron)
- C原子和单键恢复工具 (C Atom and Single Bond Restoration Tool)
- 常用基团 (Common Group)
- R基团定义工具 (R Group Definition Tool)
- 可变位置连接工具 (Variable Position Connection Tool)
- 模版工具 (Template Tool)
- 索套选择工具 (Lasso Selection Tool)
- 原子锁定工具 (Atom Locking Tool)
- 镜面旋转工具 (Mirror Rotation Tool)
- 结构检索选择 (Structure Search Selection)
- 负电子 (Negatron)
- 单双键, RS构型, 不确定键定义工具 (Single/Double Bond, RS Configuration, Uncertain Bond Definition Tool)
- 常见环, 多元环工具 (Common Ring, Polycyclic Ring Tool)

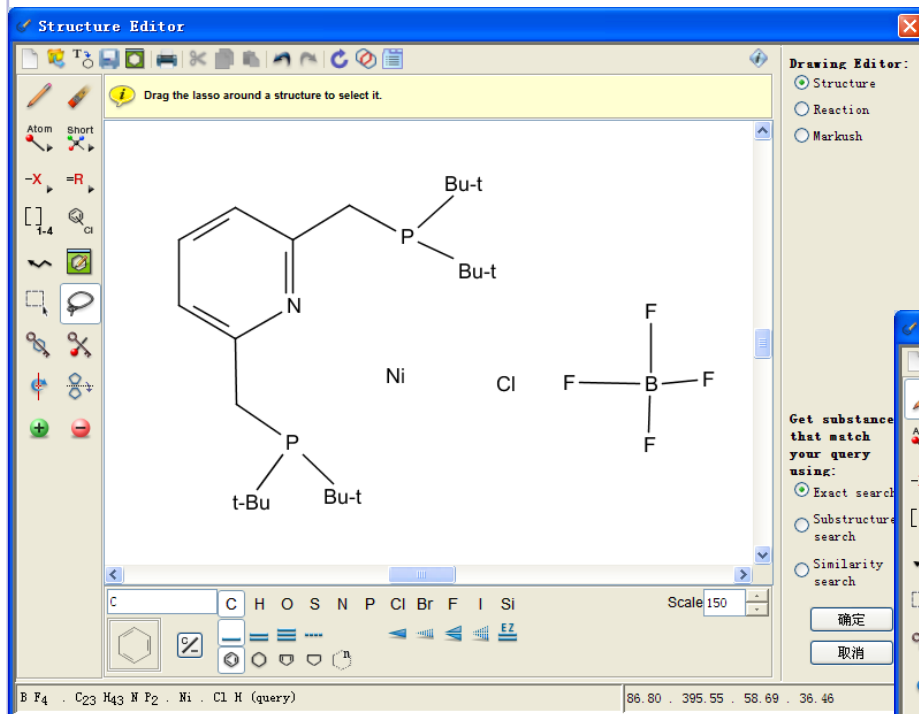
物质检索——精确结构检索



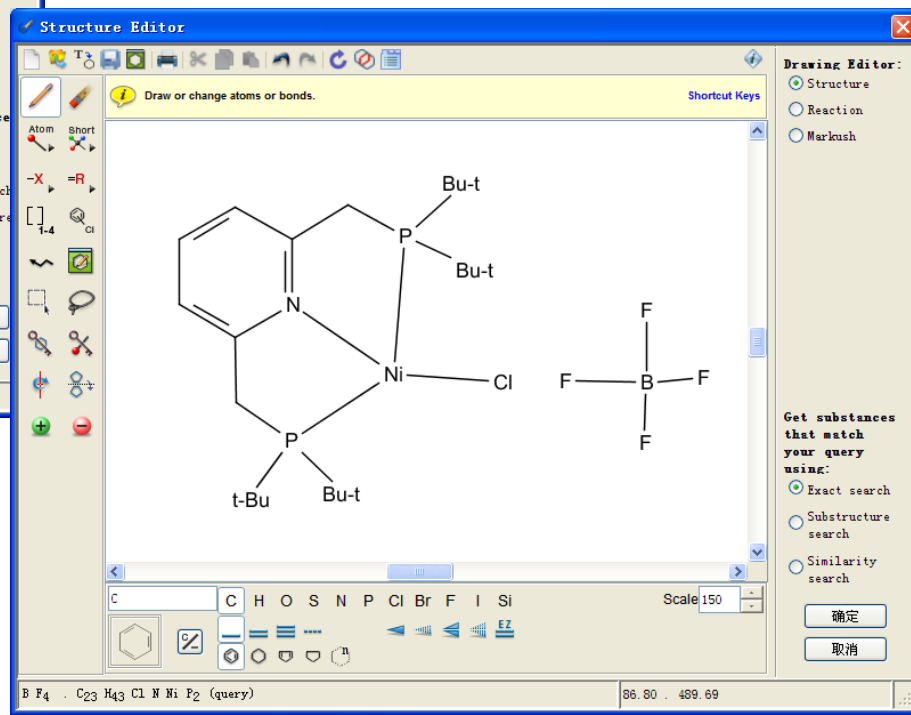
该结构中包含：

配体
金属
阳离子
阴离子

物质检索——精确结构检索



任何一种结构,使用精确结构都可以检索到



物质检索——精确结构检索

- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索

The screenshot displays the 'Structure Editor' window. The central workspace shows a chemical structure of a benzodioxane derivative with a benzene ring fused to a six-membered ring containing an oxygen atom and a carbonyl group, with a phenyl ring attached to the six-membered ring. The interface includes a toolbar on the left with various drawing tools, a top toolbar with file operations, and a right-hand panel with search options. The search options are: 'Exact search', 'Substructure search' (highlighted with a purple box), and 'Similarity search'. The bottom status bar shows the molecular formula $C_{15}H_{12}O_2$ and the molecular weight 224.26.

Structure Editor

Select and draw structures with templates.

Drawing Editor:

- Structure
- Reaction
- Markush

Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

OK

Cancel

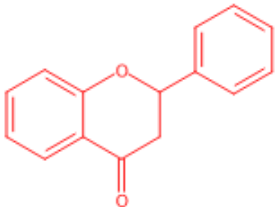
$C_{15}H_{12}O_2$ 224.26

物质检索——亚结构检索

0 of 23824 Substances Selected

1. 487-26-3

~2093

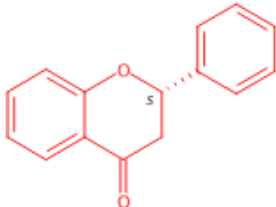


$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-2-phenyl-

▶ Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2

~244



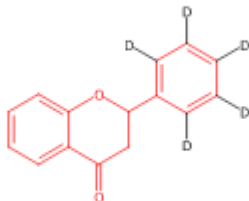
Absolute stereochemistry...Rotation (-).

$C_{15}H_{12}O_2$
4-phenyl-4H-1-benzopyran-4-one, 2,3-dihydro-

▶ Key Physical Properties
Experimental Properties

10. 146196-91-0

~1 ~5



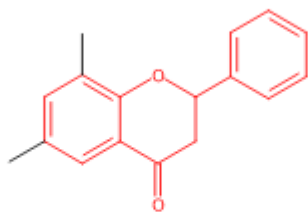
$C_{15}H_7D_5O_2$
4-(2,3,4,5-tetradeuteriophenyl)-4H-1-benzopyran-4-one, 2,3-dihydro-2-(phenyl- d_4)- (9CI)

Spectra

同位素

亚结构检索结果

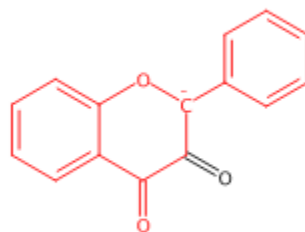
取代物



$C_{17}H_{16}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl-

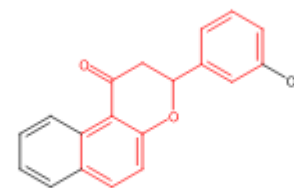
▶ **Key Physical Properties**
Experimental Properties

离子



$C_{15}H_9O_3$
2*H*-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

稠环物质



$C_{19}H_{14}O_3$
1*H*-Naphtho[2,1-*b*]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

▶ **Key Physical Properties**

亚结构检索结果的限定

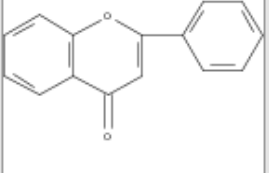
化学结构的再次限定

Analysis Refine

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Chemical Structure:

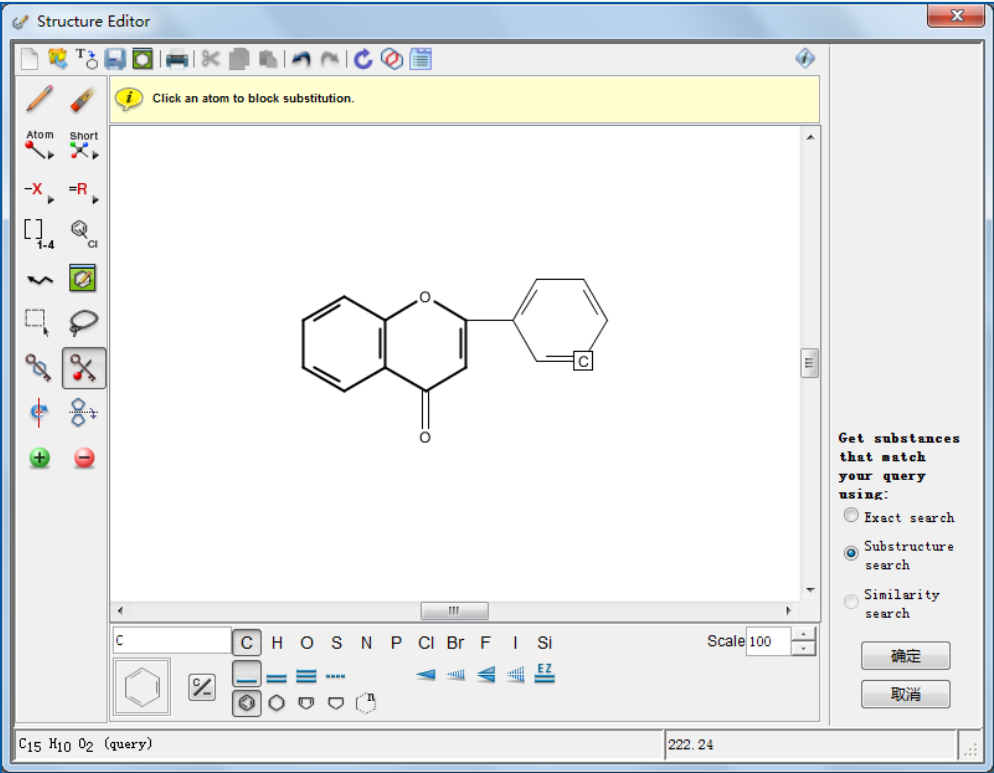


Click image to change structure or view detail

Search type: **Substructure**

Structure Editor

Click an atom to block substitution.



Get substances that match your query using:

- Exact search
- Substructure search
- Similarity search

确定 取消

C₁₅ H₁₀ O₂ (query) 222.24



环锁定

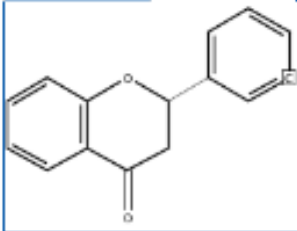


原子锁定

亚结构检索结果的限定

Structure Editor:

Java Non-Java



Click image to change structure or view detail.
Search type: **Substructure**

Only retrieve substances that:

- Have references
- Are commercially available
- Are a single component
- Are in specific substance classes
- Are in specific types of studies

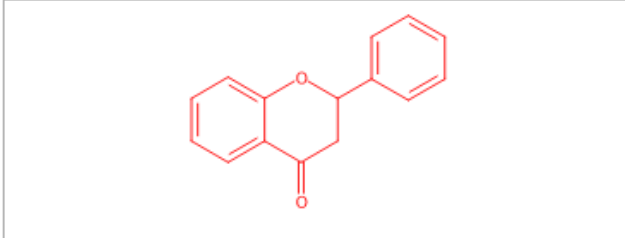
Refine

Get References Get Reactions Get Commercial Sources Tools

Sort by: Relevance

0 of 13826 Substances Selected

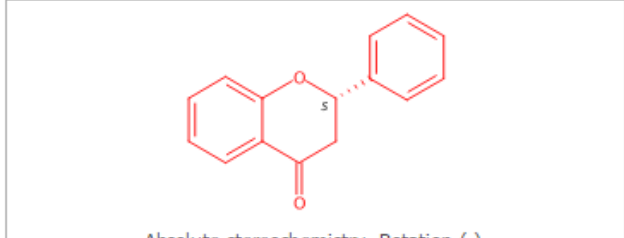
1. 487-26-3
~2093



$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-

Key Physical Properties
Regulatory Information
Spectra
Experimental Properties

2. 17002-31-2
~244



Absolute stereochemistry., Rotation (-).

$C_{15}H_{12}O_2$
4*H*-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2*S*)-

Key Physical Properties
Experimental Properties

4. 104550-32-5
~3

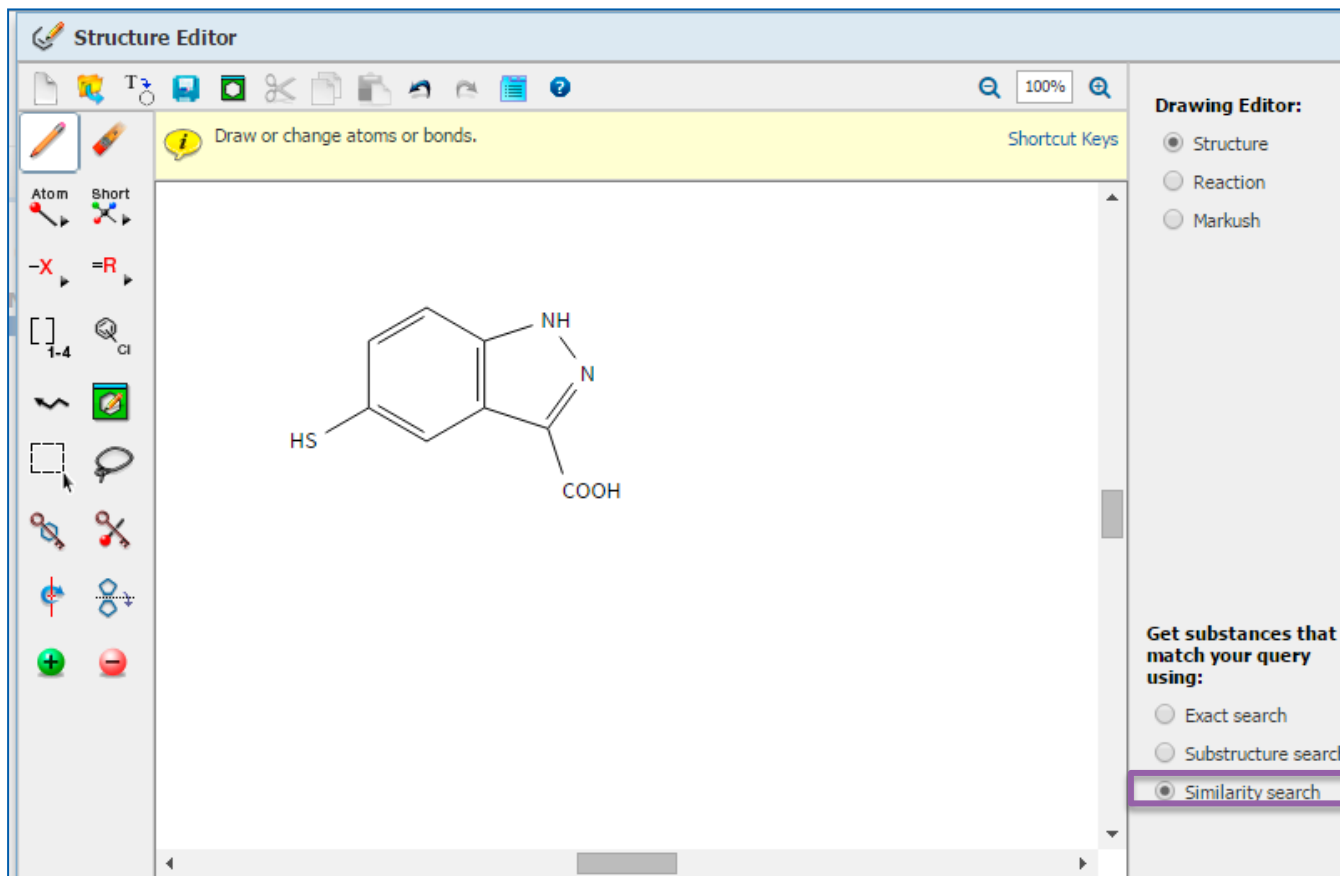
5. 75524-43-5
~2

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索



相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	11
<input type="checkbox"/> 80-84	34
<input type="checkbox"/> 75-79	84
<input type="checkbox"/> 70-74	267
<input type="checkbox"/> 65-69	696
<input type="checkbox"/> 0-64 (least similar)	1818

Get Substances

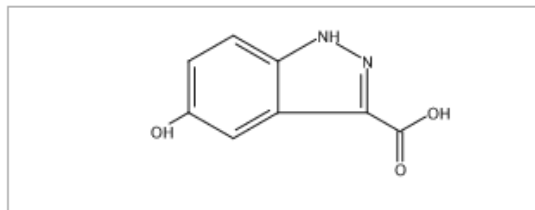
评分越高，相似度越高，结构越相似

Score: 88

1. 885518-94-5

取代基变化

~1 ~35



$C_8H_6N_2O_3$

1H-Indazole-3-carboxylic acid, 5-hydroxy-

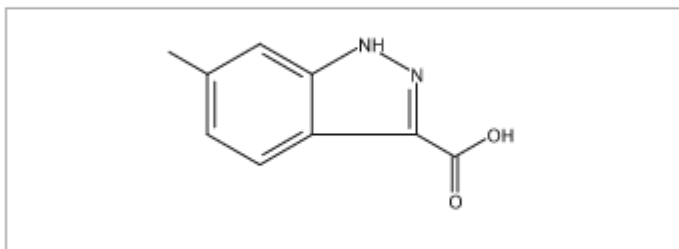
▶ Key Physical Properties

Score: 86

5. 858227-12-0

取代基位置变化

~7 ~41



$C_9H_8N_2O_2$

1H-Indazole-3-carboxylic acid, 6-methyl-

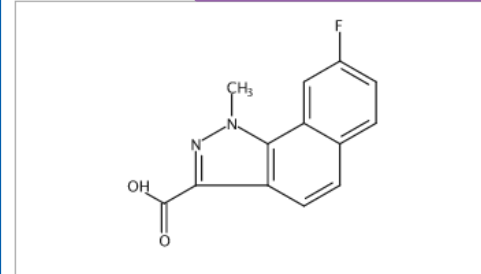
▶ Key Physical Properties

Score: 65

541. 1100422-

母体结构变化

~1



$C_{13}H_9FN_2O_2$

1H-Benz[σ]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

▶ Key Physical Properties



SCIFINDER[®]
A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

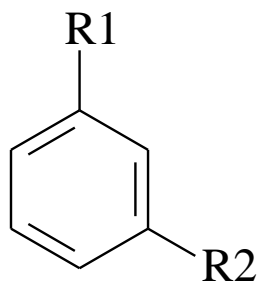
获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索 (PatentPak)
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

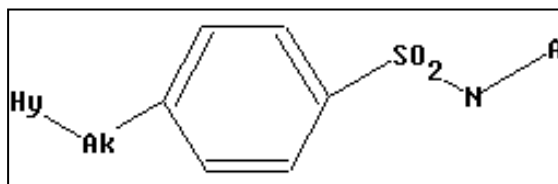
Markush检索

- 具体物质[Specific Substance] :
 - 以具体化学结构陈述的特定物质，会被分配CAS RN
- 预测性物质[Prophetic Substance] :
 - 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
 - 专利中所陈述的预测物质，不会被分配CAS RN
 - Markush检索，能检索到通过结构检索检不到的专利



R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH—halogen,
|
CH₃



可用SciFinder中的Markush检索
查看专利中化合物结构保护范围。

The screenshot shows the 'Structure Editor' window. The central canvas displays the chemical structure of the benzene ring with 'Hy-Ak' and '-SO₂-N-A' substituents. On the right, the 'Drawing Editor' panel is active, with the 'Markush' radio button selected. Below it, the 'Get Markush patents where the structure(s) are:' section has two options: 'Variable only at the specified positions' (unselected) and 'Substructures of more complex structures' (selected). At the bottom right of the panel are 'OK' and 'Cancel' buttons.

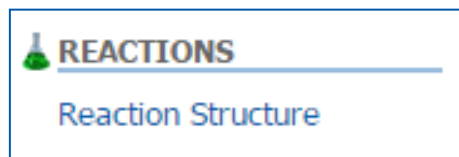
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 反应检索方法

结构式



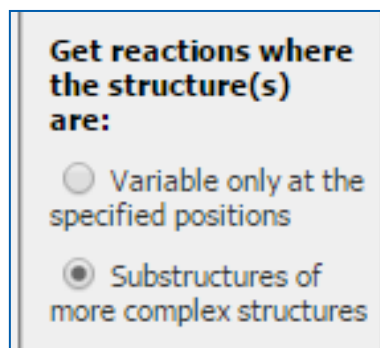
- 常用获取方法

已知物质：由物质获取反应

已知文献：从文献中获取反应

精确结构反应检索

亚结构反应检索



反应绘制工具

The screenshot shows the 'Structure Editor' window. The top toolbar includes icons for file operations and a search bar. The left sidebar contains various drawing tools. The main workspace is currently empty. The right sidebar has a 'Drawing Editor' section with radio buttons for 'Structure', 'Reaction', and 'Markush', and a section for 'Get reactions where the structure(s) are:' with radio buttons for 'Variable only at the specified positions' and 'Substructures of more complex structures'. The bottom of the window features a chemical element palette (C, H, O, S, N, P, Cl, Br, F, I, Si) and a status bar showing '16.04'.

Annotations in Chinese:

- 反应箭头 (Reaction Arrow): Points to the reaction arrow icon in the left sidebar.
- 反应原子标记工具 (Reaction Atom Marking Tool): Points to the 'A B' marking tool in the left sidebar.
- 官能团列表 (Functional Group List): Points to the 'alcohol ketone' list in the left sidebar.
- 反应角色工具 (Reaction Role Tool): Points to the reaction role icons (green and red circles) in the left sidebar.
- 反应位置标记工具 (Reaction Position Marking Tool): Points to the marking tool with a curved arrow in the left sidebar.

SciFinder反应检索——精确反应检索

The screenshot displays the SciFinder Structure Editor interface. The central workspace shows a chemical reaction: nitrobenzene (reactant) is converted to aniline (product). The reactant is a benzene ring with a nitro group (NO_2) at the para position, and the product is a benzene ring with an amino group (NH_2) at the para position. The interface includes a drawing toolbar on the left with various tools for creating and editing chemical structures. The 'Drawing Editor' panel on the right is active, showing options for 'Structure', 'Reaction', and 'Markush'. Under the 'Get reactions where the structure(s) are:' section, the 'Substructures of more complex structures' option is selected. A callout box points to this section with the text '精确反应检索' (Precise Reaction Search). The status bar at the bottom shows the molecular formula $\text{C}_7\text{H}_7\text{NO}_2 \cdot \text{C}_7\text{H}_9\text{N}$ and the reaction ID 137.14 . 107.16.

精确反应检索

反应检索结果

浏览记录，发现很多反应来自同一篇文献，
通过Group by Document合并。

1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step *Hover over any structure for more options.*

Cc1ccc([N+](=O)[O-])cc1 → Cc1ccc(N)cc1

~102 100%
~122

Overview

Steps/Stages

1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C

Notes

solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

获取相似反应

选择相似反应的相似限制：

Broad：仅反应中心相似

Medium：反应中心及附属原子和键

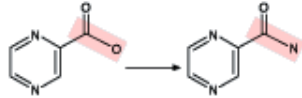
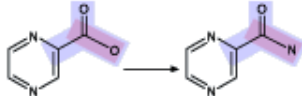
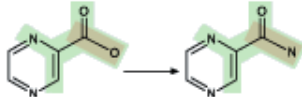
Narrow：反应中心及扩展的原子和键

Get Similar Reactions ?

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (2934)

- Medium - Reaction centers plus adjacent atoms and bonds (109)

- Narrow - Reaction centers plus extended atoms and bonds (95)


按照反应类型排序

Group by: Transformation ▾ Sort by: Frequency ▾ ↓

0 of 560 Reactions Selected

1. Reduction of Nitro Compounds to Amines
538 Reactions

$$\text{R-NO}_2 \longrightarrow \text{R-NH}_2$$

2. Reduction of Nitro to Azo Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N=N-Ar}$$

3. Reduction of Nitro to Azoxy Compounds
11 Reactions

$$\text{Ar-NO}_2 \longrightarrow \text{Ar-N}^+\text{=N-Ar} \text{O}^-$$

更精确的查找需要的反应

反应检索结果的筛选

获得特定物质做还原剂的反应

The screenshot displays the SciFinder interface for reaction search results. On the left, a sidebar titled "REACTANTS" shows a list of reagents with their respective counts. The "NaBH₄" entry is highlighted with a purple box, and a purple arrow points from this box to the text "获得特定物质做还原剂的反应".

Reagent	Count
H ₂	148
NaBH ₄	51
N ₂ H ₄ -H ₂ O	43
KOH	17
CO	16
HCO ₂ H	16
NH ₄ ⁺ •HCO ₂ ⁻	16
H ₂ O	14
N ₂ H ₄	14
NaOH	14

The main area shows a reaction detail for the reduction of 4-nitrotoluene to 4-aminotoluene. The reaction is shown as:

Cc1ccc(cc1[N+](=O)[O-])>>Cc1ccc(cc1)N

The yield is 100%. Below the reaction, the "Overview" section provides the following details:

- Steps/Stages:** 1.1 R:NaBH₄, C:1832616-28-0, C:Ru, S:H₂O, S:THF, 45 min, 25°C
- Notes:** solid-supported catalyst, ruthenium supported on porous organic polymer used, reusable catalyst, sealed tube used, scalable, Reactants: 1, Reagents: 1, Catalysts: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1
- References:** Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors

SciFinder囊括最大的反应实验过程合集

Single Step Hover over any structure for more options.



Overview

Steps/Stages

1.1 R:H₂, R:Cs₂CO₃, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

[Quick View](#) [Other Sources](#)

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

Experimental Procedure

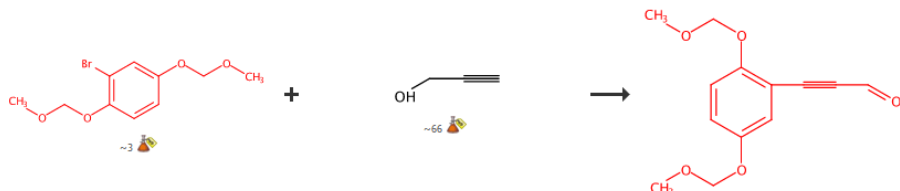


General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H₂ to a mixture of nitroarene (0.3 mmol), Cs₂CO₃ (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6 × 10⁻³ mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H₂ in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

SciFinder囊括最大的反应实验过程合集

2 Steps Hover over any structure for more options.



Overview

Steps/Stages

- 1.1 C: Pd(PPh₃)₄, S: t-BuNH₂, 21 h, 100 °C
- 2.1 R: DMSO, R: Cl(O=)CC(=O)Cl, S: CH₂Cl₂, 15 min, -78 °C
- 2.2 S: CH₂Cl₂, -78 °C; 2 h, -78 °C
- 2.3 R: Et₃N, 30 min, -78 °C; -78 °C → rt
- 2.4 R: H₂O, R: NH₄Cl, 30 min, rt

Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and temperature, Sonogashira coupling, 2) key intermediate, Swern oxidation, see method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, 5
Most stages in any one step: 4

References

Synthesis of Bioactive Speciosins G and P from *Hexagonia speciosa*
[Quick View](#) [Other Sources](#)
 By Guerrero-Vasquez, Guillermo A. et al
 From Journal of Natural Products, 77(9), 2029-2036; 2014

Experimental Procedure:

我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么?
- 查免费的Supporting Information? 可能只有图谱。

Experimental Procedure

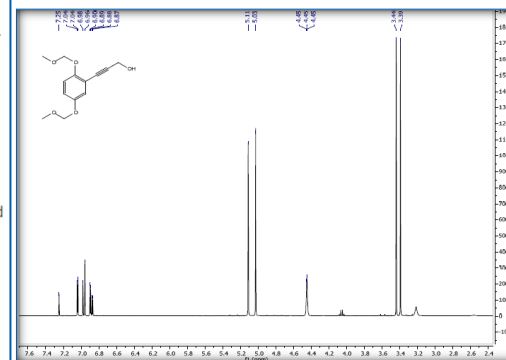


Step 1

General Procedure for the Sonogashira Coupling.^{8,10,11} Compounds **6a**³¹ and **16**⁸ were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in *n*-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in *n*-butylamine (10 mL) and Pd(Ph₃)₄ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured into H₂O (80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10–50%). *3*-(2,5-Bis(methoxymethoxy)phenyl)prop-2-yn-1-ol² (**8**). Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, *J* = 9 and 3.0 Hz, H-5), 7.03 (1H, d, *J* = 9.0 Hz, H-6), 7.10 (1H, d, *J* = 3.0 Hz, H-3); ¹³C NMR (CDCl₃, 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]⁺ (calcd for C₁₃H₁₆O₅ 275.0896).

Step 2

Generation of the Key Aldehyde.¹⁷ Oxalyl chloride (272.3 μ L, 3.12 mmol) in dry CH₂Cl₂ (9 mL) was added to a stirred solution of DMSO (332 μ L, 4.68 mmol) in dry CH₂Cl₂ (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol **8** (393.5 mg, 1.56 mmol) or alcohol **17** (300 mg, 1.56 mmol) in dry CH₂Cl₂ (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the starting material had been consumed (nearly 2 h), Et₃N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was allowed to warm to rt and quenched with saturated NH₄Cl and H₂O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH₂Cl₂ (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and evaporated under reduced pressure. *3*-(2,5-Bis(methoxymethoxy)phenyl)prop-2-ynal (**9**). Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, *J* = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, *J* = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, *J* = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ¹³C NMR (CDCl₃, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]⁺ (calcd for C₁₃H₁₄O₅ 273.0739).



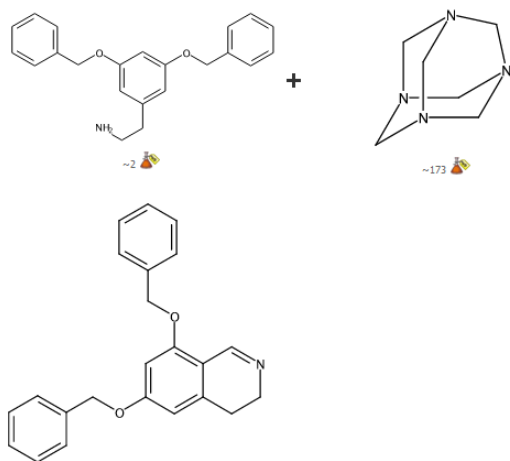
MethodsNow Synthesis

MethodsNow

Asymmetric formal synthesis of schulzeines A and C

By Jang, Jaebong; Jung, Jong-Wiha; Ahn, Jaeseung; Sim, Jaehoon; Chang, Dong-Jo; Kim, Dae-Duk; Suh, Young-Ger
 From Organic & Biomolecular Chemistry, 10(27), 5202-5204; 2012
 Published by Royal Society of Chemistry

Reaction Steps 1 2 3 4 5 6 7 8 9 10 11



多步反应中，原文没有描述
 的实验过程以灰色标示

Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	<ol style="list-style-type: none"> 1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethanamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon 2. Stir the mixture for 3 hours at 90°C. 3. Dilute the reaction mixture with H₂O. 4. Basify with potassium carbonate and extract with CH₂Cl₂. 5. Wash the combined organic layers with brine. 6. Dry over MgSO₄ and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
¹H NMR	(CDCl ₃ , 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, <i>J</i> = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
¹³C NMR	(CDCl ₃ , 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν _{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm ⁻¹
HRMS	(FAB+) calcd for C ₂₃ H ₂₂ N ₂ (M+H ⁺) 344.1651; found 344.1658
Mass Spec	(FAB+) <i>m/z</i> 344 (M+H ⁺)
State	yellow solid
CAS Method Number	3-614-CAS-200055

物质信息

实验过程

图谱信息

保存/导出方法

Print/Export Close

亚结构反应检索

通过C-H活化对苯并噻唑或者恶唑进行烷基化

The screenshot displays the Structure Editor software interface. The main workspace shows a chemical structure of benzothiazole with an R1 group attached to the 2-position. The R-group Definitions panel is open, showing a list of R-groups (R1 to R10) and a search field containing "O, S". Below the search field is a periodic table of elements with the element S (Sulfur) highlighted. The interface includes a toolbar on the left with various drawing tools, a top menu bar, and a bottom status bar indicating "Formula is not available".

Structure Editor

Draw or change atoms or bonds.

R-group Definitions

R1 R2 R3 R4 R5 R6 R7 R8 R9 R10

R1 = O, S

Atoms

H																			He
Li	Be									B	C	N	O	F					Ne
Na	Mg									Al	Si	P	S	Cl	Ar				
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	**																	
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Variables

Shortcuts

Close

Formula is not available

亚结构反应检索

The screenshot displays the Structure Editor interface. The main workspace shows a chemical reaction: a reactant (a benzimidazole ring with an R1 substituent and a hydrogen atom at the 2-position) reacting to form a product (the same benzimidazole ring with an R1 substituent and an Ak substituent at the 2-position). A purple box highlights the '-X' button in the left toolbar, with an arrow pointing to the 'Variables' panel on the right. The 'Variables' panel lists search filters: X (Any halogen), M (Any metal), A (Any atom except H), Q (Any atom except C or H), Ak (Any carbon chain), Cy (Any cycle), Cb (Any carbocycle), and Hy (Any heterocycle). The 'Drawing Editor' panel is set to 'Reaction'. The 'Get reactions where the structure(s) are:' panel has 'Substructures of more complex structures' selected. The bottom status bar shows 'Formula is not available'.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Drawing Editor:

- Structure
- Reaction
- Markush

Variables

- X Any halogen
- M Any metal
- A Any atom except H
- Q Any atom except C or H
- AK** Any carbon chain
- Cy Any cycle
- Cb Any carbocycle
- Hy Any heterocycle

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures

Formula is not available

亚结构反应检索

The screenshot displays the Structure Editor software interface. The main workspace shows a chemical reaction: a benzimidazole derivative with a substituent R1 and a hydrogen atom on the imidazole ring (labeled 'reactant') reacts to form the same derivative with a substituent R1 and a substituent Ak on the imidazole ring (labeled 'product').

On the right side, the Drawing Editor panel is visible, with the 'Reaction' radio button selected. Below it, the search criteria are set to 'Substructures of more complex structures', which is highlighted with a purple box.

At the bottom of the interface, there is a toolbar with various drawing tools and a list of elements: C, H, O, S, N, P, Cl, Br, F, I, Si. A search bar contains the text 'Ak'. The status bar at the bottom left indicates 'Formula is not available'.

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应

Analyze Refine

Analyze by: ?
Catalyst

CuI	28
312696-09-6	17
AgNO ₃	17
(MeOCH ₂ CH ₂) ₂ O	16
NaI	15
1905414-33-6	14
CoBr ₂	11
Me ₃ SiCH ₂ MgCl	10
Ph ₂ P(CH ₂) ₃ PPh ₂	10
658062-48-7	9

Group by: No Grouping Sort by: Accession Number

No Grouping
Document
Transformation

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

~57 ~52 83%

Overview

Steps/Stages

- 1.1 R:LiO-Bu-*t* C:1905414-33-6, S:Dioxane, 16 h, 100°C
- 1.2 S:H₂O, rt
- 1.3 R:HCl, S:H₂O, neutralized

Notes

catalyst prepared and used, screw cap tube used, Reactants: 2, Reagents: 2, Catalysts: 1, Solvents: one step: 3

References

ACS / Proprietary and Confidential / Do Not Distribute

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciPlanner使用简介

3. View Reaction Detail [Link](#) **勾选想要的反应**

3 Steps *Hover over any structure for more options.* **点击Send to SciPlanner** [Display Options](#)

Overview

Steps/Stages

- 1.1 R: NH₃, R: t-BuOK, R: t-BuOOH, S: THF
- 2.1 R: NaH, S: THF
- 3.1 R: POCl₃, reflux

Notes

Reactants: 2, Reagents: 5, Solvents: 1, Steps: 3, Stages: 3, Most stages in any one step: 1

References

Syntheses of 4- and 6-substituted thiazolo[4,5-c]pyridines

进入SciPlanner 新建文件

SciPlanner SciPlanner_11_19_2015_112612 **将刚推送过来的反应拖至编辑面板**

Workspace Edit View GoTo

- New
- Open
- Save
- Duplicate
- Import
- Export
- Print
- Close

Your Workspace is empty.

Drag items from the reference, substance, and reaction libraries (on the right) to this area.

SciPlanner使用简介

SciPlanner 11_19_2015_112612

Workspace Edit View GoTo

CAS Registry Number: 13091-23-1

- View Substance Detail
- Explore by Structure
- Synthesize this...
- Get Reactions where Substance is a
- Get Commercial Sources
- Get Regulatory Information
- Get References
- Export as Image
- Export as molfile

打开中间产物的标准菜单
选择Synthesis this

1 2 3

Get References Tools

Send selected records to SciPlanner. Send to SciPlanner

Group by: No Grouping Sort by: Accession Number

1 of 34 Reactions Selected

1. View Reaction Detail

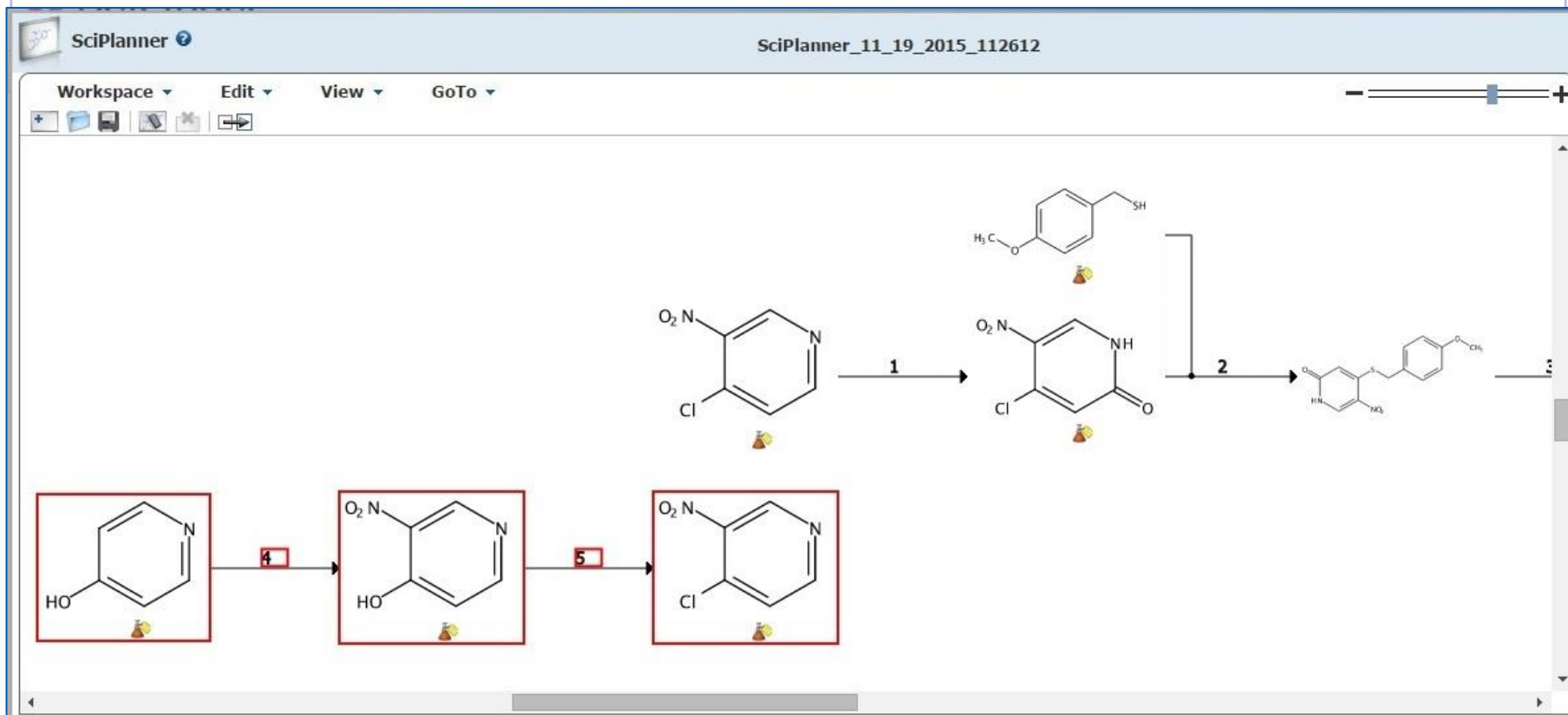
2 Steps Hover over any structure for more options.

在检索到的反应中选择感兴趣的反应

继续推送到SciPlanner

~161 ~192

SciPlanner使用简介

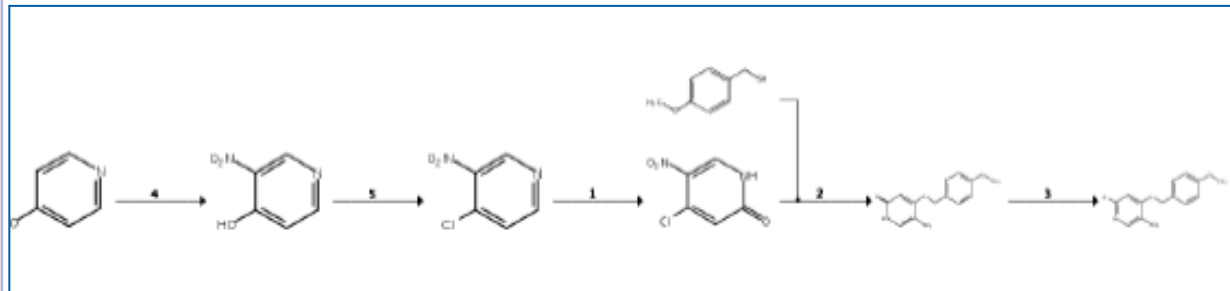


步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

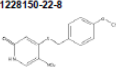
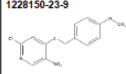
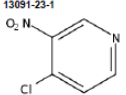
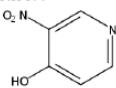
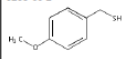
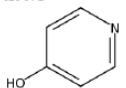
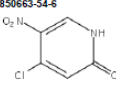
SciPlanner使用简介

The screenshot displays the SciPlanner software interface. At the top, the title bar reads "SciPlanner" and "SciPlanner_11_19_2015_112612". Below the title bar is a menu bar with "Workspace", "Edit", "View", and "GoTo". A "Workspace" dropdown menu is open on the left, listing options: "New", "Open", "Save", "Duplicate", "Import", "Export", "Print", and "Close". The "Export" option is highlighted in blue. In the center, a chemical reaction scheme is shown with three pyridine rings. The first ring has a nitro group (O₂N) and a hydroxyl group (HO). An arrow labeled "4" points to the second ring, which has a nitro group (O₂N) and a chlorine atom (Cl). An arrow labeled "5" points to the third ring, which also has a nitro group (O₂N) and a chlorine atom (Cl). An arrow labeled "1" points to a fourth structure, which is a pyridine ring with a nitro group (O₂N) and a chlorine atom (Cl), and a side chain consisting of a double bond to a carbon atom, which is further bonded to a chlorine atom (Cl) and a methyl group (H₃C). A pink callout box with a pointer to the "Export" menu item contains the text: "点击 Workspace, 选择 Export 导出结果". Another pink callout box with a pointer to the second and third pyridine rings contains the text: "用鼠标将两个同样的结构拖至重叠, 两条反应合并". A third pink callout box with a pointer to the "Export" dialog box contains the text: "选择适当的输出格式, 输出结果". The "Export" dialog box is open on the right, titled "Export". It has a "For:" section with "Offline Review" selected. Under "Offline Review", there are three radio buttons: "Portable Document Format (*.pdf)", "Citations (*.ris)", and "Image (*.png)". There is also a "Saving Locally" section with a radio button for "SciPlanner eXchange (*.pkx)". The "Details:" section includes a "File Name:" field with the text "SciPlanner_11_19_2015_112612" and a "Title" field. The "Include:" section has four checked checkboxes: "SciPlanner Image", "Reaction Details", "Substance Details", and "Reference Details". At the bottom right of the dialog box are "Export" and "Cancel" buttons.

SciPlanner导出结果



Reaction	Stages	Notes	Yield
5	<p>1.1 R:POCl₃, S:PhMe, 0°C → rt; 16 h, rt → 110°C</p> <p>1.2 R:K₂CO₃, S:H₂O, cooled, pH 10</p>	<p>Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2</p> <p>Transformation:</p> <p>1. Formation of Alkyl Halides from Alcohols</p>	90%
<p>References</p> <p>High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes</p> <p>By Poloek, Anurach et al</p> <p>From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014</p>			

Substance Information		
<p>1228150-22-8</p>  <p>C₁₃H₁₂N₂O₄S 2-(1<i>H</i>)-Pyridinone, 4-[[[4-(methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>1228150-23-9</p>  <p>C₁₃H₁₁ClN₂O₃S Pyridine, 2-chloro-4-[[[4-(methoxyphenyl)methyl]thio]-5-nitro-</p> <p>Related Info: ~ 2 References Reactions</p>	<p>13091-23-1</p>  <p>C₅H₃ClN₂O₂ Pyridine, 4-chloro-3-nitro-</p> <p>Related Info: ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information</p>
<p>5435-54-1</p>  <p>C₅H₄N₂O₂ 4-Pyridinol, 3-nitro-</p> <p>Related Info: ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information</p>	<p>6258-60-2</p>  <p>C₈H₁₀O S Benzenemethanethiol, 4-methoxy-</p> <p>Related Info: ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information</p>	<p>626-64-2</p>  <p>C₅H₄N O 4-Pyridinol</p> <p>Related Info: ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information</p>
<p>850663-54-6</p>  <p>C₆H₃ClN₂O₃ 2-(1<i>H</i>)-Pyridinone, 4-chloro-5-nitro-</p> <p>Related Info: ~ 22 References Reactions ~ 136 Commercial Sources</p>		

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - **MethodsNow**
- SciFinder常见问题及解决

MethodsNow™ 是一个完整的 CAS 解决方案



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- Pharmacology / Toxicology: 成瘾药物检测，有毒物检测...
- Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定...
- Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析...
- Historical Analysis / Dating: 考古分析，同位素分析
- Environmental Analysis: 土壤/空气/水分析，农药残留分析...
- Agricultural Applications / Analysis: 除草剂分析...
- Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析...
- Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工...
- Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析...

目前有13个大类，45个小类。某些子项目属于多种方法分类

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方法分类



历史检索



The screenshot shows the MethodsNow website interface. At the top, there is a navigation bar with the logo 'METHODSNOW A CAS SOLUTION' and links for 'Saved' and 'Account'. Below the navigation bar is a search section with the heading 'Search' and a search input field. A callout bubble points to the search input field with the text '保存结果集'. Below the search input field is a link for 'Advanced Search'. The main content area is titled 'Browse Method Categories' and lists various categories such as 'Agricultural Applications / Analysis', 'Bioassays', 'Biomolecule Isolation', 'Environmental Analysis', 'Food Analysis', 'Organic Compound Analysis', 'Pharmacology / Toxicology', 'Polymer Analysis', and 'Water Analysis'. A callout bubble points to the 'Organic Compound Analysis' category with the text '点击一个类别 浏览相关方法'. Below the categories is a section for 'Recent Searches' with a list of search terms, including 'hplc lycopene analysis'. A callout bubble points to the 'hplc lycopene analysis' entry with the text '点击历史检索 重新运行检索'. Another callout bubble points to the 'X' icon next to the search term with the text '点击“X” 删除检索历史'.

高级检索

The image shows two overlapping screenshots of the CAS MethodsNow Advanced Search interface. The top screenshot shows the main search area with a 'Keyword' field and a dropdown menu for logical operators. A callout box points to the operator dropdown with the text '逻辑运算符 : and, or, not'. Another callout box points to a close button on the right with the text '删除检索条件'. The bottom screenshot shows the 'Add Search Criteria' dropdown menu open, listing search options: Keyword, Analyte, Matrix, Method Category, Technique, CAS Method Number, and Publication Name. A callout box points to this menu with the text '检索选项 : 关键词、分析物、基质、方法分类、技术、CAS Method Number、期刊名'. The interface includes the 'METHODSNow' logo, 'CAS SOLUTION' text, and user options for 'Saved' and 'Account'.

CAS Solutions

METHODSNow™
A CAS SOLUTION

★ Saved 👤 Account

← Return to Home

Advanced Search

逻辑运算符 : and, or, not

Keyword

AND Matrix

AND Analyte

Add Search Criteria

增加检索条件

删除检索条件

CAS Solutions

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← Return to Home

Advanced Search

检索选项 : 关键词、分析物、
基质、方法分类、技术、CAS
Method Number、期刊名

Publication Name

Keyword

Analyte

Matrix

Method Category

Technique

CAS Method Number

Publication Name

案例：利用超临界萃取法分析叶片中的酚类物质

CAS Solutions



Search

此处只需输入一个关键词即可，MethodsNow会自动进行同义词查找

Enter keyword, matrix, analyte, etc.

supercritical



supercritical extraction

supercritical fluid chromatographic chiral stationary phases

supercritical fluid chromatography

Browse Method Categories

Agricultural Applications / Analysis

Fuels / Geology / Biofuels

Pharmacology / Toxicology

Bioassays

Historical Analysis / Dating

Polymer Analysis

Biomolecule Isolation

Miscellaneous

Water Analysis

Environmental Analysis

Organic Compound Analysis

Food Analysis

Organometallics / Inorganics

Recent Searches

supercritical extraction



member



结果显示

典型分析方法标题格式：通过某技术手段在某基质中分析某物质

限定分析物、
基质、方法
等条件

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METHODS NOW
A CAS SOLUTION

"supercritical extraction"

Results (581)

Sort Relevance

导出方法

保存方法

View Details & Instructions

查看方法详情

Add to Compare

方法对比

Return to Home

Analyte

- Phenols (115)
- Palmitic acid (64)
- Limonene (60)
- Myrcene (59)
- (±)- α -Pinene (55)
- View All

Matrix

- Leaf (87)
- Root (31)
- Zingiber officinale (28)
- Seed (26)
- Coffee products (21)
- View All

Method Category

Technique

- Supercritical extraction (561)
- Gas chromatography (476)

Analysis of Lutein A in Pharmaceutical natural products by HPLC
CAS MN: 1-131-CAS-120642

View Details & Instructions

Add to Compare

Analyte	Rubixanthin; Lutein A; Zeaxanthin; <i>cis</i> - β -Carotene; β -Carotene; Carotenes
Matrix	Rosa canina; Pharmaceutical natural products
Other Materials	Reagent: Ethanol; Hexane Material: Spherisorb column (5 μ m, 4.6 x 250 mm, ODS1); Stainless steel column; Glass beads (1 mm diameter) View All
Method Category	Natural Product Isolation Analysis
Technique	Liquid chromatography spectrometric detectors; HPLC; Supercritical extraction
Equipment Used	HPLC system; Diode array detector (DAD); Supercritical extraction apparatus; Thermostatic chamber

结果显示

Analysis of Phenols in *Calophyllum brasiliense* by Supercritical extraction

CAS MN: 2-105-CAS-52171

Method Category: Antioxidant Assay

Technique: Spectrophotometry; Soxhlet extractor; **Supercritical extraction**

Materials	Role	Image	CAS RN
Mammea A/BB	analyte	View Structure	6916-62-7
Xanthone	analyte	View Structure	90-47-1
Coumarin	analyte	View Structure	91-64-5
Phenols	analyte		
Biflavonoids	analyte		
<i>Calophyllum brasiliense</i>	matrix		
Leaf	matrix		
Sieves (30 and 50 mesh)	material		
Dichloromethane	reagent	View Structure	75-09-2
Methanol	reagent	View Structure	67-56-1
DPPH radical	reagent	View Structure	1898-66-4

实验材料

Source

Comparing conventional and **supercritical extraction** of (-)-mammea A/BB and the antioxidant activity of *Calophyllum brasiliense* extracts

Goncalves, Renata Menoci; Lemos, Caroline Ortega Terra; Leal, Ivana Correa Ramos; Nakamura, Celso Vataru; Cortez, Diogenes Aparicio Garcia; da Silva, Edson Antonio; Cabral, Vladimir Ferreira; Cardozo-Filho, Lucio

Molecules (2013), 18, 6215 - 6229. MDPI AG

CODEN: MOLEFW | ISSN: 14203049 | DOI: 10.3390/molecules18066215

[Document Sources](#)

Abstract ^

Calophyllum brasiliense is a rich source of bioactive coumarins, xanthones and biflavonoids. The aim of the study was to compare the phenol contents and the antioxidant activity of *C. brasiliense* extracts obtained by conventional and supercritical fluid extraction (SFE) methods, as well as the quantification of crude extracts and (-)-mammea A/BB yields. Dichloromethane and hexane were used as solvents for the conventional extractions and SFE was developed using supercritical CO₂; the kinetic curves were modeled using a second-order empirical model. The dichloromethane extract presented the best total yield, although it showed the lowest content of (-)-mammea A/BB. The concentration of the coumarin was considerably higher in concerning the ed to be more

Instructions

Organic solvent extraction using Soxhlet apparatus

1. Collect the leaves of *Calophyllum brasiliense* Cambess.
2. Dry the plant material in a circulating air oven (QUIMIS Q-31) at 313 K temperature.
3. Mill the leaves in a home processor (WALITA RI7625) after 72 h.
4. Use Tyler sieves (W. S. Tyler, Mentor, OH, USA) to classify the samples according to particle size.
5. Select the leaves trapped in the 30 and 50 mesh sieves for the extraction.
6. Perform the organic solvent extraction for 300 min using a Soxhlet apparatus.
7. Use dichloromethane as a solvent due to the differences in terms of polarity and dielectric constant.
8. Set the boiling point at 313 K and the dielectric constant at 8.93.
9. Express the yields obtained for each solvent extraction and calculate in relation to the initial dry weight sample.

Determination of antioxidant activity by DPPH (2,2-diphenyl-1-picrylhydrazyl) method

1. Dilute the extracts in methanol up to concentrations from 25 to 350 µg/mL.
2. Add 2,850 µl of the DPPH solution (0.6 mM) to 150 µL of sample.
3. Substitute the volume of the samples by distilled water for the blank control.
4. Keep the reaction for 1 h at room temperature, in the dark.
5. Measure the absorbance at 515 nm.
6. Express the antioxidant activity (AA%) as a percentage of DPPH radical elimination, calculate according to the following equation: $AA\% = [(1 - A_{sample})/A_{blank}] \times 100$, where A.blank represents the absorbance of the blank and A.sample represents the absorbance of the extract solution.
7. Calculate the concentration of the extracts resulting in 50% of inhibition (IC₅₀) from the inhibition percentage plotting graph.

Validation

Inhibitory Activity 206.58 µg/mL (IC₅₀)

文献信息

Equipment Used

Oven, Q-31, QUIMIS

Processor, RI7625, WALITA

Spectrophotometer, UV-1203, Shimadzu

Conditions

Instrument

Detection wavelength - 515 nm

设备条件

实验步骤及数据有效性

对比不同分析方法

导出对比
PDF文件

	1	2	3
Title	Analysis of Phenols in <i>Calophyllum brasiliense</i> by Supercritical extraction	Analysis of Phenols in <i>Calophyllum brasiliense</i> by Supercritical extraction	Analysis of Phenols in <i>Calophyllum brasiliense</i> by Supercritical extraction
CAS Method Number	2-105-CAS-52171	1-131-CAS-62310	1-131-CAS-52140
Method Category	Antioxidant Assay	Natural Product Isolation	
Technique	Spectrophotometry; Soxhlet extractor; Supercritical extraction	Spectrophotometry; Soxhlet extraction	
Analyte	Mammea A/BB; Xanthone; Coumarin; Phenols; Biflavonoids	Phenols	
Matrix	<i>Calophyllum brasiliense</i> ; Leaf	<i>Calophyllum brasiliense</i> ; Leaf	
Other Materials	Dichloromethane; Methanol; DPPH radical; Sieves (30 and 50 mesh)	Methanol; Sodium carbonate; Folin-Ciocalteu (30 and 50 mesh)	
Equipment Used	Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu	Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu; Syringe pumps.	Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu; Syringe pumps.
Conditions	Instrument: Detection wavelength - 515 nm	Instrument: Detection wavelength - 760 nm	Instrument: Detection wavelength - 760 nm
Source	Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant	Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant	Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant
Method	Organic solvent extraction using Soxhlet apparatus 1. Collect the leaves of <i>Calophyllum brasiliense</i> Cambout	Supercritical Fluid Extraction (SFE) 1. Collect the leaves of <i>Calophyllum brasiliense</i> Cambout	Supercritical Fluid Extraction (SFE) 1. Collect the leaves of <i>Calophyllum brasiliense</i> Cambout
Inhibitory Activity	206.58 µg/mL (IC ₅₀)		
Concentration		26.98 ± 2.90 mg of GAE/g of extract	15.06 ± 1.75 mg of GAE/g of extract

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
 - 文献检索
 - 物质检索
 - Markush检索
 - 反应检索 (MethodsNow Synthesis)
 - SciPlanner
 - MethodsNow
- SciFinder常见问题及解决

SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

如何获取SciFinder账号

The screenshot displays the SciFinder registration interface, divided into three main sections:

- CONTACT INFORMATION--**: Includes input fields for First Name, Last Name, Email, Confirm Email, Phone Number, and Fax Number. It also features dropdown menus for Area of Research and Job Title.
- USERNAME AND PASSWORD--**: Includes input fields for Username (with a 'Tips' link), Password, and Re-enter Password.
- SECURITY INFORMATION--**: Includes a dropdown menu for Security Question and an input field for Answer (with a 'Why?' link).

At the bottom of the form, there are two buttons: 'Register>>' and 'Clear All'.

请注意：

1. 必须输入真实姓名和**学校域名**邮箱。
2. 用户名必须是唯一的，且包含 5-15 个字符。它可以只包含字母或字母组合、数字和/或以下特殊字符：

- - (破折号)
- _ (下划线)
- . (句点)
- @ (表示“at”的符号)

3. 密码必须包含 7-15 个字符，并且至少**包含三种以下字符**：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符 (例如 @、#、%、&、*)

例：abc@123

4. 从下拉列表中选择一个密码提示问题并给出答案。
单击 Register (注册)。

如何获取SciFinder账号

From: CAS

Dear user,

To complete your SciFinder registration, you must click the link provided below. By clicking the link, you agree to all of the following terms and conditions:

- I will not share my username and password with any other person.
- I will search only for myself and not for others or other organizations.
- I will not use any automated program or script for extracting or downloading CAS data, or any other systematic retrieval of data.
- I may retain a maximum of 5,000 Records at any given time for personal use or to share within a Project team for the duration of the Project.
- My organization's SciFinder License and the CAS Information Use Policies (<http://www.cas.org/legal/infopolicy.html>) apply to my use of SciFinder.
- I will contact my SciFinder Key Contact if I have questions.

If you do not accept these terms and conditions, do not click the link and delete this e-mail message.

<https://scifinder.cas.org/registration/completeRegistration.html?respKey=B8CB6727-86F3-F014-11E6-D312D80AC094>

This link is valid for only one use and will expire within 48 hours.

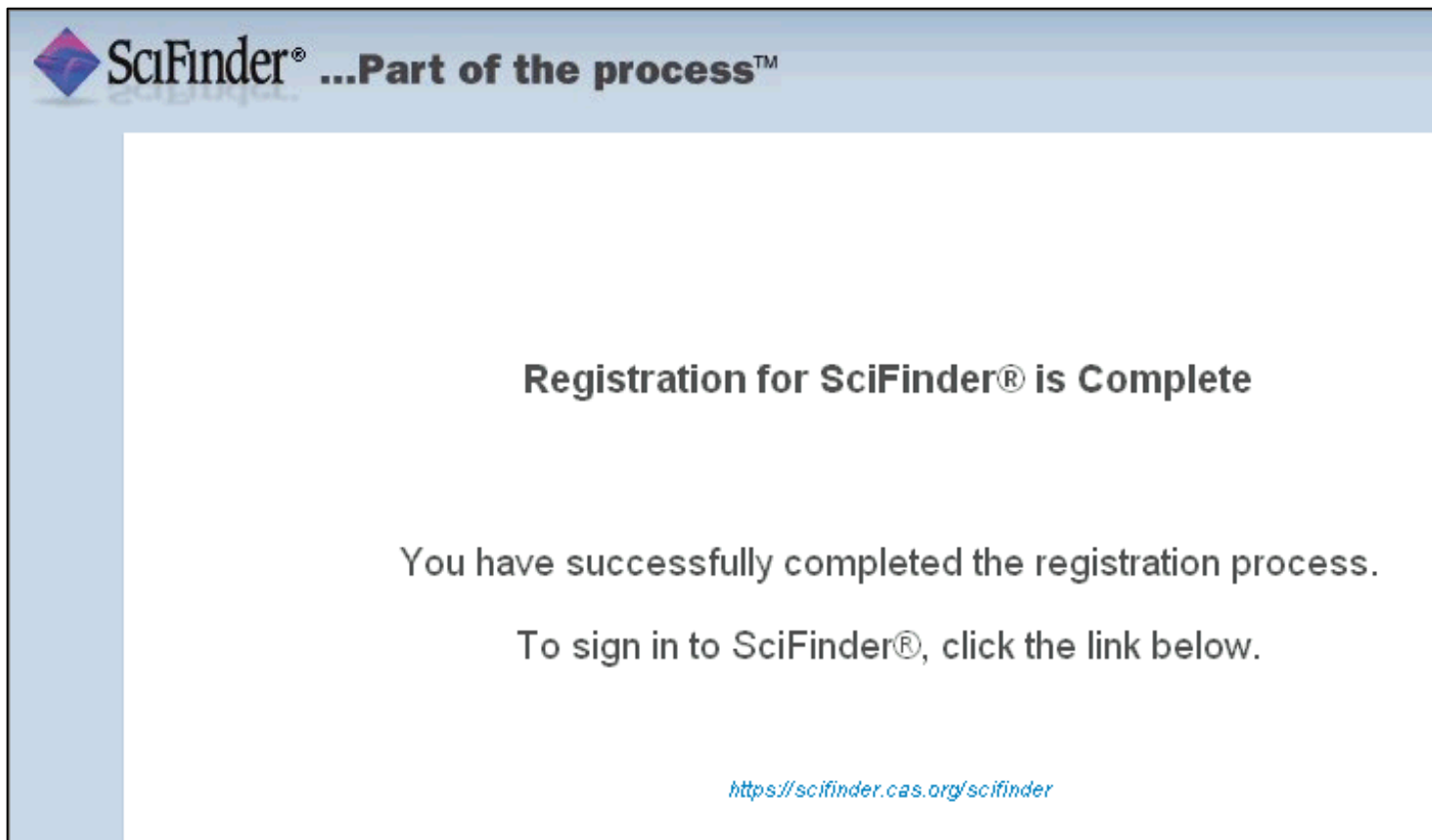
If you need assistance at any time, consult the key contact at your organization.

打开并阅读 CAS 的电子邮件（必须在48小时内点击，否则需要重新注册）

注意垃圾邮件、未知邮件、订阅邮件等来自@cas.org的邮件



如何获取SciFinder账号



账号注册成功，登录scifinder.cas.org开始使用SciFinder

SciFinder使用注意事项

- 一人注册一个帐号
- 请提供真实姓名信息
- 严禁过量下载
- 严禁账号分享
- 严禁将账号用于非学术研究

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